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Supporting Material

**DNA Sequence-directed Organization of Chromatin: Structure-based
Computational Analysis of Nucleosome-binding Sequences**

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Supplementary Materials

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Sreekala Balasubramanian, Fei Xu, and Wilma K. Olson

Department of Chemistry & Chemical Biology

Rutgers, the State University of New Jersey

Wright-Rieman Laboratories

610 Taylor Road

Piscataway, New Jersey 08854-8087, USA

List of Supplementary Tables

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|------------------|--|
| Table S1. | Protein-DNA complexes with resolution $\leq 2.5 \text{ \AA}$ used to generate knowledge-based potentials. |
| Table S2. | Nucleosome-positioning sequences: (i) nucleosome-binding sequences from the mouse genome; (ii) anti-selection sequences from the mouse genome; (iii) synthetic SELEX sequences; (iv) high-resolution positioning sequences. |
| Table S3. | Properties of DNA base-Pair steps used in knowledge-based potentials: (i) number of base-pair steps included in derived ‘energy’ functions; (ii) average values and dispersion of Tilt, $\langle \theta_1 \rangle \pm (\sigma_{\theta_1})$, in protein-bound DNA dimers; (iii) average values and dispersion of Roll, $\langle \theta_2 \rangle \pm (\sigma_{\theta_2})$, in protein-bound DNA dimers; (iv) average values and dispersion of Twist, $\langle \theta_3 \rangle \pm (\sigma_{\theta_3})$, in protein-bound DNA dimers; (v) average values and dispersion of Shift, $\langle \theta_4 \rangle \pm (\sigma_{\theta_4})$, in protein-bound DNA dimers; (vi) average values and dispersion of Slide, $\langle \theta_5 \rangle \pm (\sigma_{\theta_5})$, in protein-bound DNA dimers; (vii) average values and dispersion of Rise, $\langle \theta_6 \rangle \pm (\sigma_{\theta_6})$, in protein-bound DNA dimers; (viii) relative base-pair flexibility V of protein-bound DNA dimers. |
| Table S4. | Comparative ‘cost’ of nucleosomal deformation of individual base-pair steps with knowledge-based functions based on different subsets of observed protein-bound DNA conformations: (i) pyrimidine-purine (YR) base-pair steps; (ii) purine-purine and pyrimidine-pyrimidine (RR, YY) base-pair steps; (iii) purine-pyrimidine (RY) base-pair steps. |
| Table S5. | Threading scores of known nucleosome-binding and nucleosome-resistant sequences on the central 60 base-pair steps of the 147-bp nucleosome core-particle structure (NDB_ID pd0287) (2) and an ideal 61-bp superhelical template with the same average global structure. |

Table S1. Protein-DNA complexes with resolution $\leq 2.5 \text{ \AA}$ used to generate knowledge-based potentials.

| NDB_ID | PDB_ID | Structure Description | Resol. (\text{\AA}) | Literature citation |
|--------|--------|---|------------------------|-------------------------------------|
| PD0002 | 1A73 | INTRON-ENCODED ENDONUCLEASE I-PPOI/DNA COMPLEX | 1.8 | Flick <i>et al.</i> , 1998 |
| PD0003 | 1CRX | CRE RECOMBINASE/DNA COMPLEX | 2.4 | Guo <i>et al.</i> , 1997 |
| PD0006 | 3PVI | RESTRICTION ENDONUCLEASE PVUII/DNA COMPLEX | 1.59 | Horton <i>et al.</i> , 1998b |
| PD0007 | 9ANT | ANTENNAPEPIDA HOMEODOMAIN/DNA COMPLEX | 2.4 | Fraenkel & Pabo, 1998 |
| PD0008 | 1A6Y | REVERBA ORPHAN NUCLEAR RECEPTOR/DNA COMPLEX | 2.3 | Zhao <i>et al.</i> , 1998 |
| PD0010 | 1BGB | ECORV ENDONUCLEASE/DNA COMPLEX | 2.0 | Horton & Perona, 1998a |
| PD0011 | 2PVI | RESTRICTION ENDONUCLEASE/DNA COMPLEX | 1.76 | Horton <i>et al.</i> , 1998a |
| PD0012 | 1BNZ | SSO7D HYPERTHERMOPHILE PROTEIN/DNA COMPLEX | 2.0 | Gao <i>et al.</i> , 1998 |
| PD0013 | 1RV5 | ECORV ENDONUCLEASE/DNA COMPLEX | 2.1 | Horton & Perona, 1998b |
| PD0016 | 3HDD | ENGRAILED HOMEODOMAIN/DNA COMPLEX | 2.2 | Fraenkel <i>et al.</i> , 1998 |
| PD0020 | 1BC8 | SAP-1 ETS DOMAIN/DNA COMPLEX | 1.9 | Mo <i>et al.</i> , 1998 |
| PD0024 | 1B3T | EBNA-1 NUCLEAR PROTEIN/DNA COMPLEX | 2.2 | Bochkarev <i>et al.</i> , 1998 |
| PD0027 | 1BC7 | SERUM RESPONSE FACTOR ACCESSORY PROTEIN 1A (SAP-1)/DNA COMPLEX | 2.0 | Mo <i>et al.</i> , 1998 |
| PD0028 | 1BG1 | TRANSCRIPTION FACTOR STAT3B/DNA COMPLEX | 2.2 | Becker <i>et al.</i> , 1998 |
| PD0029 | 2BAM | PROTEIN (ENDONUCLEASE BAMHI)/DNA COMPLEX | 2.0 | Viadiu & Aggarwal, 1998 |
| PD0030 | 2KTQ | LARGE FRAGMENT OF DNA POLYMERASE I/DNA COMPLEX | 2.3 | Li <i>et al.</i> , 1998b |
| PD0031 | 3BAM | PROTEIN (RESTRICTION ENDONUCLEASE BAMHI) (3.1.21.4)/DNA COMPLEX | 1.8 | Viadiu, & Aggarwal, 1998 |
| PD0032 | 3KTQ | LARGE FRAGMENT OF DNA POLYMERASE I/DNA COMPLEX | 2.3 | Li <i>et al.</i> , 1998b |
| PD0033 | 4KTQ | LARGE FRAGMENT OF DNA POLYMERASE I/DNA COMPLEX | 2.5 | Li <i>et al.</i> , 1998b |
| PD0035 | 1BDT | WILD TYPE GENE-REGULATING PROTEIN ARC/DNA COMPLEX | 2.5 | Schildbach <i>et al.</i> , 1999 |
| PD0037 | 1B94 | RESTRICTION ENDONUCLEASE ECORV/DNA COMPLEX | 1.9 | Thomas <i>et al.</i> , 1999 |
| PD0042 | 1B8I | IV/HOMEobox PROTEIN EXTRADENTICLE/DNA COMPLEX PRE-TRANSITION STATE ECO RI | 2.4 | Passner <i>et al.</i> , 1999 |
| PD0049 | 1CKQ | ENDONUCLEASE/DNA COMPLEX | 1.85 | Horvath <i>et al.</i> , unpublished |
| PD0050 | 6PAX | HOMEobox PROTEIN PAX-6/DNA COMPLEX | 2.5 | Xu <i>et al.</i> , 1999 |
| PD0051 | 1CKT | HIGH MOBILITY GROUP PROTEIN HMG1/DNA COMPLEX | 2.5 | Ohndorf <i>et al.</i> , 1999 |

| NDB_ID | PDB_ID | Structure Description | Resol. (Å) | Literature citation |
|--------|--------|---|---------------|-------------------------------------|
| PD0052 | 1SSP | URACIL-DNA GLYCOSYLASE/DNA COMPLEX | 1.9 | Parikh <i>et al.</i> , 1998 |
| PD0054 | 1CL8 | ENDONUCLEASE/DNA COMPLEX | 1.8 | Horvath <i>et al.</i> , unpublished |
| PD0055 | 1QPS | ENDONUCLEASE ECORI/DNA COMPLEX | 2.5 | Horvath <i>et al.</i> , unpublished |
| PD0056 | 1QPZ | PURINE NUCLEOTIDE SYNTHESIS REPRESSOR/DNA COMPLEX | 2.5 | Glasfeld <i>et al.</i> , 1999 |
| PD0062 | 1QRH | RESTRICTION ENDONUCLEASE ECO-RI/DNA COMPLEX | 2.5 | Choi <i>et al.</i> , 2002 |
| PD0065 | 1QSY | KLENOW FRAGMENT OF DNA POLYMERASE I/DNA COMPLEX | 2.3 | Li <i>et al.</i> , 1999 |
| PD0066 | 1QSS | KLENOW FRAGMENT OF DNA POLYMERASE I/DNA COMPLEX | 2.3 | Li <i>et al.</i> , 1999 |
| PD0067 | 1QTM | DNA POLYMERASE I (E.C.2.7.7.7)/DNA COMPLEX | 2.3 | Li <i>et al.</i> , 1999 |
| PD0068 | 1QUM | ENDONUCLEASE IV (E.C.3.1.21.2)/DNA COMPLEX | 1.6 | Hosfield <i>et al.</i> , 1999 |
| PD0070 | 1D3U | TATA-BINDING PROTEIN/DNA COMPLEX | 2.4 | Littlefield <i>et al.</i> , 1999 |
| PD0071 | 1BY4 | PROTEIN RETINOIC ACID RECEPTOR/DNA COMPLEX | 2.1 | Zhao <i>et al.</i> , 2000 |
| PD0073 | 3HTS | HEAT SHOCK TRANSCRIPTION FACTOR/DNA COMPLEX | 1.8 | Littlefield & Nelson, 1999 |
| PD0075 | 1B72 | PBX1, HOMEOBOX PROTEIN HOX-B1/DNA TERNARY COMPLEX | 2.4 | Piper <i>et al.</i> , 1999 |
| PD0076 | 2IRF | INTERFERON REGULATORY FACTOR 2/DNA COMPLEX | 2.2 | Fujii <i>et al.</i> , 1999 |
| PD0088 | 1BF4 | PROTEIN (CHROMOSOMAL PROTEIN SSO7D)/DNA COMPLEX | 1.6 | Gao <i>et al.</i> , 1998 |
| PD0089 | 1HWT | PROTEIN (HEME ACTIVATOR PROTEIN)/DNA COMPLEX | 2.5 | King <i>et al.</i> , 1999a |
| PD0090 | 2HAP | HEME ACTIVATOR PROTEIN HAP1-18/DNA COMPLEX | 2.5 | King <i>et al.</i> , 1999b |
| PD0096 | 1CYQ | INTRON-ENCODED HOMING ENDONUCLEASE I-PPOI/DNA COMPLEX | 1.9 | Galburt <i>et al.</i> , 1999 |
| PD0099 | 1DIZ | 3-METHYLADENINE DNA GLYCOSYLASE II/DNA COMPLEX | 2.5 | Hollis <i>et al.</i> , 2000 |
| PD0101 | 1DFM | ENDONUCLEASE BGLII/DNA COMPLEX | 1.5 | Lukacs <i>et al.</i> , 2000 |
| PD0108 | 1DMU | BGLI RESTRICTION ENDONUCLEASE/DNA COMPLEX | 2.2 | Newman <i>et al.</i> , 1998 |
| PD0110 | 1QRV | HIGH MOBILITY GROUP PROTEIN D/DNA COMPLEX | 2.2 | Murphy IV <i>et al.</i> , 1999 |
| PD0111 | 1DP7 | MHC CLASS II TRANSCRIPTION FACTOR HRFX1/DNA COMPLEX | 1.5 | Gajiwala <i>et al.</i> , 2000 |
| PD0115 | 1DSZ | RETINOIC ACID RECEPTOR RXR α & RAR α /DNA COMPLEX | 1.7 | Rastinejad <i>et al.</i> , 2000 |
| PD0116 | 1DUX | ETS-DOMAIN PROTEIN ELK-1/DNA COMPLEX | 2.1 | Mo <i>et al.</i> , 2000 |
| PD0117 | 1EBM | 8-OXOGUANINE DNA GLYCOSYLASE/DNA COMPLEX | 2.1 | Bruner <i>et al.</i> , 2000 |
| PD0119 | 1CA5 | CHROMOSOMAL PROTEIN SAC7D/DNA COMPLEX | 2.2 | Su <i>et al.</i> , 2000 |
| PD0120 | 1CA6 | CHROMOSOMAL PROTEIN SAC7D/DNA COMPLEX | 2.2 | Su <i>et al.</i> , 2000 |
| PD0121 | 1EGW | MADS BOX TRANSCRIPTION ENHANCER FACTOR 2/DNA COMPLEX | 1.5 | Santelli & Richmond, 2000 |
| PD0122 | 1QPI | TETRACYCLINE REPRESSOR/DNA COMPLEX | 2.5 | Orth <i>et al.</i> , 2000 |

| NDB_ID | PDB_ID | Structure Description | Resol. (Å) | Literature citation |
|---------|--------|--|---------------|-------------------------------------|
| PD0126 | 1QAI | REVERSE TRANSCRIPTASE/DNA COMPLEX | 2.3 | Najmudin <i>et al.</i> , 2000 |
| PD0127 | 1EMH | URACIL-DNA GLYCOSYLASE/DNA COMPLEX | 1.8 | Parikh <i>et al.</i> , 2000 |
| PD0131 | 1EON | TYPE II RESTRICTION ENZYME ECORV/DNA COMPLEX | 1.6 | Horton <i>et al.</i> , 2000 |
| PD0132 | 1EOO | TYPE II RESTRICTION ENZYME ECORV/DNA COMPLEX | 2.2 | Horton & Perona, 2000 |
| PD0139 | 1ESG | TYPE II RESTRICTION ENZYME BAMH/DNA COMPLEX | 1.9 | Viadiu & Aggarwal, 2000 |
| PD0141 | 1EWN | 3-METHYL-ADENINE DNA GLYCOSYLASE/DNA COMPLEX | 2.1 | Lau <i>et al.</i> , 2000 |
| PD0142 | 1EWQ | DNA MISMATCH REPAIR PROTEIN MUTS/DNA COMPLEX | 2.2 | Obmolova <i>et al.</i> , 2000 |
| PD0147 | 1EYU | TYPE II RESTRICTION ENZYME PVUII/DNA COMPLEX | 1.8 | Horton & Cheng, 2000 |
| PD0151 | 1D02 | RESTRICTION ENDONUCLEASE/DNA COMPLEX | 1.7 | Deibert <i>et al.</i> , 1999 |
| PD0152 | 1D1U | MOLONEY MURINE LEUKEMIA VIRUS REVERSE TRANSCRIPTASE/DNA COMPLEX | 2.3 | Cote <i>et al.</i> , 2000 |
| PD0153 | 1D2I | RESTRICTION ENDONUCLEASE BGLI/DNA COMPLEX | 1.7 | Lukacs <i>et al.</i> , 2000 |
| PD0154 | 1QN4 | TRANSCRIPTION INITIATION FACTOR TFIID-1/DNA COMPLEX | 1.9 | Patikoglou <i>et al.</i> , 1999 |
| PD0160 | 1QNA | TRANSCRIPTION INITIATION FACTOR TFIID-1/DNA COMPLEX | 1.8 | Patikoglou <i>et al.</i> , 1999 |
| PD0173 | 1MJ2 | METHIONINE REPRESSOR MUTANT (Q44K)/DNA COMPLEX | 2.4 | Garvie & Phillips, 2000 |
| PD0180 | 1GD2 | TRANSCRIPTION FACTOR PAP1/DNA COMPLEX | 2.0 | Fujii <i>et al.</i> , 2000 |
| PD0194 | 1FJX | HHAI METHYLTRANSFERASE MUTANT | 2.3 | Vilkaitis <i>et al.</i> , 2000 |
| PDE001 | 1ERI | ECO RI ENDONUCLEASE (E.C.3.1.21.4)/DNA COMPLEX | 2.5 | Kim <i>et al.</i> , 1990 |
| PDE005 | 1DNK | (E.C.3.1.21.1)/DNA COMPLEX | 2.3 | Weston <i>et al.</i> , 1992 |
| PDE006 | 2DNJ | (E.C.3.1.21.1)/DNA COMPLEX | 2.0 | Lahm & Suck, 1991 |
| PDE009 | 1HCR | HIN RECOMBINASE/DNA COMPLEX | 2.3 | Feng <i>et al.</i> , 1994 |
| PDE0125 | 1BPY | DNA POLYMERASE β/DNA COMPLEX | 2.2 | Sawaya <i>et al.</i> , 1997 |
| PDE0126 | 1BPX | DNA POLYMERASE β/DNA COMPLEX | 2.4 | Sawaya <i>et al.</i> , 1997 |
| PDE0128 | 1TC3 | TC3 TRANSPOSEASE/DNA COMPLEX | 2.5 | Van Pouderoyen <i>et al.</i> , 1997 |
| PDE0131 | 2BDP | DNA POLYMERASE I/DNA COMPLEX | 1.8 | Kiefer <i>et al.</i> , 1998 |
| PDE0132 | 3BDP | DNA POLYMERASE I/DNA COMPLEX | 1.9 | Kiefer <i>et al.</i> , 1998 |
| PDE0133 | 4BDP | DNA POLYMERASE I/DNA COMPLEX | 1.8 | Kiefer <i>et al.</i> , 1998 |
| PDE0135 | 1T7P | DNA POLYMERASE, THIOREDOXIN/DNA COMPLEX | 2.2 | Doublie <i>et al.</i> , 1998 |
| PDE014 | 1RVA | ECO RV/DNA COMPLEX | 2.0 | Kostrewa & Winkler, 1995 |
| PDE0143 | 1A35 | HUMAN TOPOISOMERASE I/DNA COMPLEX | 2.5 | Redinbo <i>et al.</i> , 1998 |

| NDB_ID | PDB_ID | Structure Description | Resol. (Å) | Literature citation |
|---------|--------|---|---------------|---------------------------------|
| PDE0145 | 1BSU | ENDONUCLEASE ECORV (E.C.3.1.21.4)/DNA COMPLEX | 2.0 | Martin <i>et al.</i> , 1999 |
| PDE020 | 1BHM | BAMHI (E.C.3.1.21.4)/DNA COMPLEX | 2.2 | Newman <i>et al.</i> , 1995 |
| PDE025 | 1FJL | SEGMENTATION PROTEIN PAIRED/DNA COMPLEX | 2.0 | Wilson <i>et al.</i> , 1995 |
| PDE139 | 1AZ0 | ECORV ENDONUCLEASE (E.C.3.1.21.4)/DNA COMPLEX | 2.0 | Perona & Martin, 1997 |
| PDE141 | 6MHT | CYTOSINE-SPECIFIC METHYLTRANSFERASE HHAI (E.C.2.1.1.73)/DNA COMPLEX | 2.05 | Kumar <i>et al.</i> , 1997 |
| PDR001 | 3CRO | 434 CRO/DNA COMPLEX | 2.5 | Mondragon & Harrison, 1991 |
| PDR004 | 2OR1 | 434 REPRESSOR/DNA COMPLEX | 2.5 | Aggarwal <i>et al.</i> , 1988 |
| PDR010 | 1LMB | LAMBDA REPRESSOR/DNA COMPLEX | 1.8 | Beamer & Pabo, 1992 |
| PDR011 | 1RPE | 434 REPRESSOR/DNA COMPLEX | 2.5 | Shimon & Harrison, 1993 |
| PDR013 | 1TRR | TRP REPRESSOR/DNA COMPLEX | 2.4 | Lawson & Carey, 1993 |
| PDR015 | 1PER | 434 REPRESSOR/DNA COMPLEX | 2.5 | Rodgers & Harrison, 1993 |
| PDR018 | 1PDN | PRD PAIRED/DNA COMPLEX | 2.5 | Xu <i>et al.</i> , 1995 |
| PDR021 | 2NLL | RETINOIC ACID RECEPTOR, THYROID HORMONE RECEPTOR/DNA COMPLEX | 1.9 | Rastinejad <i>et al.</i> , 1995 |
| PDR022 | 1TSR | P53 TUMOR SUPPRESSOR/DNA COMPLEX | 2.2 | Cho <i>et al.</i> , 1994 |
| PDR023 | 1BER | CAP/DNA COMPLEX | 2.5 | Parkinson <i>et al.</i> , 1996 |
| PDR031 | 1AIS | TATA-BINDING PROTEIN/DNA COMPLEX | 2.1 | Kosa <i>et al.</i> , 1997 |
| PDR032 | 1A3Q | HUMAN NF-κB P52 BOUND TO DNA | 2.1 | Cramer <i>et al.</i> , 1997 |
| PDR034 | 1AU7 | PIT-1 MUTANT/DNA COMPLEX | 2.3 | Jacobson <i>et al.</i> , 1997 |
| PDR036 | 1MNM | α-2 TRANSCRIPTIONAL REPRESSOR/DNA COMPLEX | 2.2 | Tan & Richmond, 1998 |
| PDR047 | 1AZP | HYPERTHERMOPHILE CHROMOSOMAL PROTEIN SAC7D/DNA COMPLEX | 1.6 | Robinson <i>et al.</i> , 1998 |
| PDR048 | 1AZQ | HYPERTHERMOPHILE CHROMOSOMAL PROTEIN SAC7D/DNA COMPLEX | 1.9 | Robinson <i>et al.</i> , 1998 |
| PDR049 | 1AKH | MAT A1/ α2/DNA TERNARY COMPLEX | 2.5 | Li <i>et al.</i> , 1998a |
| PDR051 | 2RAM | TRANSCRIPTION FACTOR NF-κB P65/DNA COMPLEX | 2.4 | Chen <i>et al.</i> , 1998 |
| PDR056 | 1BL0 | MULTIPLE ANTIBIOTIC RESISTANCE PROTEIN/DNA COMPLEX | 2.3 | Rhee <i>et al.</i> , 1998 |
| PDRC03 | 1HCQ | ESTROGEN RECEPTOR/DNA COMPLEX | 2.4 | Schwabe <i>et al.</i> , 1993 |
| PDT012 | 1YTB | TATA BINDING PROTEIN (TBP)/DNA COMPLEX | 1.8 | Kim <i>et al.</i> , 1993 |
| PDT013 | – | HNF-3/FORK HEAD DNA-RECOGNITION MOTIF/DNA COMPLEX | 2.5 | Clark <i>et al.</i> , 1993 |

| NDB_ID | PDB_ID | Structure Description | Resol. (Å) | Literature citation |
|--------|--------|--|---------------|-------------------------------------|
| PDT015 | 1NFK | NUCLEAR FACTOR κB (NF-κB)/DNA COMPLEX | 2.3 | Ghosh <i>et al.</i> , 1995 |
| PDT028 | 1YRN | MAT A1 HOMEODOMAIN, MAT α2 HOMEODOMAIN/DNA COMPLEX | 2.5 | Li <i>et al.</i> , 1995 |
| PDT029 | 2DGC | GCN4/DNA COMPLEX | 2.2 | Keller <i>et al.</i> , 1995 |
| PDT030 | 1LAT | GLUCOCORTICOID RECEPTOR MUTANT/DNA COMPLEX | 1.9 | Gewirth & Sigler, 1995 |
| PDT031 | – | EVEN-SKIPPED HOMEODOMAIN/DNA COMPLEX | 2.0 | Hirsch & Aggarwal, 1995 |
| PDT033 | 1PUE | TRANSCRIPTION FACTOR PU.1/DNA COMPLEX | 2.1 | Kodandapani <i>et al.</i> , 1996 |
| PDT034 | 1CDW | TATA BINDING PROTEIN (TBP)/DNA COMPLEX | 1.9 | Nikolov <i>et al.</i> , 1996 |
| PDT035 | 1IGN | RAP1/DNA COMPLEX | 2.2 | Koenig <i>et al.</i> , 1996 |
| PDT036 | 1YTF | TRANSCRIPTION FACTOR IIA (TFIIA)/DNA COMPLEX | 2.5 | Tan <i>et al.</i> , 1996 |
| PDT038 | 1UBD | YY1 ZINC FINGER DOMAIN MUTANT/DNA COMPLEX | 2.5 | Houbaviy <i>et al.</i> , 1996 |
| PDT039 | 1AAY | ZIF268 ZINC FINGER PEPTIDE/DNA COMPLEX | 1.6 | Elrod-Erickson <i>et al.</i> , 1996 |
| PDT040 | 1IHF | INTEGRATION HOST FACTOR/DNA COMPLEX | 2.2 | Rice <i>et al.</i> , 1996 |
| PDT043 | 2HDD | ENGRAILED HOMEODOMAIN Q50K VARIANT/DNA COMPLEX | 1.9 | Tucker-Kellogg <i>et al.</i> , 1997 |
| PDT044 | 1ZME | PROLINE UTILIZATION TRANSCRIPTION ACTIVATOR (PUT3)/DNA COMPLEX | 2.5 | Swaminathan <i>et al.</i> , 1997 |
| PDT045 | 1XBR | T DOMAIN/DNA COMPLEX | 2.5 | Muller & Herrmann, 1997 |
| PDT048 | 1AWC | GA BINDING PROTEIN α, GA BINDING PROTEIN β1/DNA COMPLEX | 2.1 | Batchelor <i>et al.</i> , 1998 |
| PDT049 | 2CGP | CATABOLITE GENE ACTIVATOR PROTEIN/DNA COMPLEX | 2.2 | Passner & Steitz, 1997 |
| PDT055 | 1A1F | THREE-FINGER ZIF268 PEPTIDE/DNA COMPLEX | 2.1 | Elrod-Erickson <i>et al.</i> , 1998 |
| PDT056 | 1A1G | THREE-FINGER ZIF268 PEPTIDE/DNA COMPLEX | 1.9 | Elrod-Erickson <i>et al.</i> , 1998 |
| PDT057 | 1A1H | QGSR (THREE-FINGER ZIF268 VARIANT)/DNA COMPLEX | 1.6 | Elrod-Erickson <i>et al.</i> , 1998 |
| PDT059 | 1A1I | ZINC FINGER/DNA COMPLEX | 1.6 | Elrod-Erickson <i>et al.</i> , 1998 |
| PDT062 | 1AM9 | STEROL REGULATORY ELEMENT BINDING(STRE)/DNA COMPLEX | 2.3 | Parraga <i>et al.</i> , 1998 |
| PDTB41 | 1MEY | CONSENSUS ZINC FINGER/DNA COMPLEX | 2.2 | Kim & Berg, 1996 |
| PDV001 | 2BOP | E2/DNA COMPLEX | 1.7 | Hegde <i>et al.</i> , 1992 |

Note: Multiple entries of *Eco* RV endonuclease reflect different structures solved to study the different functional aspects of the catalytic activity of the enzyme.

References to Table S1

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Table S2. Nucleosome-positioning sequences

(i) Nucleosome-binding sequences from the mouse genome
SET 1A A-tracts 1 (90%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|--------|---|
| phcn4 | 122 bp | TAGGACCTGG AGTATGGCGA GAAAAGTGA AATCACAGAA AATGAGAAAT ACACACTTTA GGATGTGAAA TATGGCGAGG AAAACTGAAA AAGGTGGAAA ATTCAAGAAAT GTCCACTGTGTA GG |
| phcn8 | 127 bp | AGGACCTGGA ACATGGTGAG AAAACTGAAA ATCACAGAAA ATGAGAAATA GACACTTTAG GACGTGAAAT ATGACGAGGA AAACAGAAAA AGTTGGAAAA TTTAGAAATG TCTAACGTAG GACGTGG |
| phcn12 | 123 bp | TGAAGGACCT GGAATATGGC GACGGAAAC TGAAAATCAC GGAAAATGAG AAATACACAC TTTACGACGT GAAATATGGC GAGGAAACACT GATAAAGGTG GAATATTTAG AAACGTCCAC TGT |
| phcn14 | 125 bp | AGGGACATGG AATATGGAGA GAAAAGTGA AATCACGGAA AATGAAAAAT ACACACTTTA GGACGTGAAA TATAGCGAGG AAAACTGAAA AAGGTGGAAAT ATTTAGAAAT GTCCACTGTGTA GGACG |
| phcn17 | 120 bp | CCGGAATATG GCGAGAAAC TGAAAATCAC GTAAAATGAG AAATACACAC TTTAGGACGT GAGATATCGC GAGGAAACCT GAAAAGGTG GAAAATTTAG AAATGTCACA GTAGGACGTG |
| phcn18 | 125 bp | TGACCTGGAA TATGGCGAGA AACCTGAAAA TCACGCAAAA TGAGAAATAC ACACTTCTAGG ACATGAAATA TGGTGAGGAA AATTGAAAAA GGTGGAATAT TAAGAAATGT CCACTGTAGG ACGTG |
| phcn21 | 129 bp | TGAAGGACCT GGAATATGGC GAGAGAACTG AAAATCACCG AAAATGAGAA ATACACACTT TAGGACGTGA AATATGGCGA GGAAAATCTGA AAAAGATGGAA AAATTTAGAA ATATCCACTG TAGGACGTG |
| phcn22 | 118 bp | AATGTGGCGA GAAAAGTGA AATCACGGAA AATGAGAAAT AAACACTTTA GGAAGTGAAA TATGGCGAGG AAAACTGAAA AGGATGGAAA ATTTAGAAAT GTCCACTGTGTA GGACGTGG |
| phcn23 | 125 bp | GAGGACCTGG AATATGGTG AAGACTGAA AATCACGGAA AATGAGAAAT ACACACTTTT GGACGTGAAA TATGGCGAGG AAAACTGAAA AAGGTGGAAA ATTTAGAAAT GTCCACTGTGTA GGACG |
| phcn24 | 111 bp | AGAGAAAACC GAAAATCACG GAAAATGAGA AATACGCAC TTAGGACGTG AAATATGGCG AGGAAAATG AAAAAGGTGG AAAATTTAGG GATGTCCACT GTAGGACGTG G |
| phcn26 | 127 bp | AGGACCTGGA ACATGGCGAG AAAACTGAAG ATCACGGAAA ATGAGAAATA CACACTTAG GGCCTGAAAT ATGACGAGGA AAACAGAAAA AGGTGGAGAA TTTAGAAATG TCCACTGTAG GACGTGG |

| | | |
|--------|--------|--|
| phcn29 | 120 bp | GGAATATGGC GAGAAAACAG AAAATCACGG GAAATGAGAA ATACACACTT TAGGACGTGA AATATAGCGA GGGGAACTGA AAAAGGTGGA AAATTAGAA ATGTCCGCTG TAGGACGTGG |
| phcn39 | 128 bp | AGAGGACCTG GAATATGGCG AGAAAACGTGA AAATCACCGA AAATGAGAAA TACACACTTT AGGACATGAA ATATGGCGAG GAAAACGTGAA AAAGGTGGAA AATTGAGAAA TGCCACTGTGTA GGACGTGG |
| phcn43 | 119 bp | AGGACCTGGA ATATGGCGAG AAAACTGAAA ATCACGGAAA ATGAGAAACA CGCGCTTAAG GACATGAAAT ATGGCGAGAA AAACGTGAAAA AGGTGGAATA TATAGAAATG TCCACTGTGTA |
| phcn46 | 126 bp | ATGCACACTG TAGGACCTGG AATATGGCGA GAAAACGTGAA AATTAAGGAA AATGAGAAAT ATACACTTTA GGACGTGAAA TATGGCGAGG AGGACTGAAA GAGGTGGAAA ATTTAGATAC GTCCAC |
| phcn47 | 128 bp | AAGGACCTGG AATATGACGA GAAAACGTGAA AATCACGGAAA AATGAGAGAT ACACACTTTA GGACGTGAAA TATGGCGAGG AAAACTGAAA AGGTGGAAGA ATTTAGAAAT GTCCACCGTA GACGTGG |
| phcn50 | 109 bp | AGAGAACTGA AAATCACCGA AAATGAGAAA TACACGCTTT AGGACGTGAA ATATGGCGAG GAAAACGTGAA AAAGGTGGAAA ATTTAGAAAT GTCCACTGTGTA GGACGTGGT |
| phwn12 | 126 bp | GACCTGGAAA ATGGCGAGAA AACTGAAAAT CACGGAAAAT GTGAAATACA CACTTTAGGA CATGAAATAT GGCGAGGAAA ATTGAAAAAG TTGGATAATT TAGAAATGTC CACTGTAGGA CGTGGA |

SET 1B A-tracts 2 (81%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|---------------------|---|
| phcn2 | 126 bp | TAGGACGTGG AATATGGCAA GAAAAGTCAA AATCATGGAA AATGATAAGC ATCCACTTGA CGACTTGAAA AATGACGAAA TCACTAAAAA ACGTAAAAAA TGAGAAATGC ACAGTGGAGG ACCTGG |
| phcn10 | 125 bp | AGAACGTGGA ATAAGGCAAG GAAACGGAAA ATCATGGAAA ATGAGGAACA TCCAATTGAC GACTGGAAA ATGACGAAAT CACTAAAAAA CGTAAAAAT GAGAAATGGA CACTGAAGGA CCTGG |
| phcn13 | 119 bp [†] | AGGACGTGAA ATTGGCGAGA AACTGGAAAG GTGGAATATT TAGAGATGTG CACTGTAGGA CGTGGAAATAT GGCAAGAAAG TGAAAAGCAT GGAAAATGAG AACACATCCAC TTGACGATT |
| phcn20 | 126 bp | TAGGACGTGG AATATGGCAA GAAAAGTCAA AATCATGGAA AATGAGAAC ATCCACTTGA TGACTTGAAA AATGACGAAA TCACTAAAAA ACGTAAAAAA TGAGAAATGC ACAGTGAAGG ACCTGA |
| phcn30 | 126 bp | TGACGACTTG AAAAATGACG AGATCACTAA AAAATGTGAA AAATGAGAAA TGCACACTGA AGGAGCTGGA ATATGGTGGG AAAACTGGAA ATTACGGAAA ATGAGAAATA CACACTTTAG GACGTG |
| phcn42 | 126 bp | AGGACGTGGG AGTATGGCAA GAAAAGTCAA AGTCATGGAA AGTGAGAAC ATCCACTTGA TGACTTGAAA AATGACGAAA TCACTGGAAAG ACGTAAAAAA TGAGAAATGCA CACTGTAGGA CATGGA |
| phwn8 | 119 bp | ATGGCAAGAA AACTGAAAAT CATGGAAAAT GAGAAACATC CACTCGACGA CTTGAAGAT GACGAAATCA CTAGAAAACG TGAAAATGA GAAATGCTCA CTGAAGGACC TGAATATGG |
| phwn26 | 124 bp | TAGGACGTGG AATATGGCAA GAAATCTGAA AATCATGGAA AATGAGAAC ATCCACTTGA TGACTTGAAA ATGACGAAAT CACTAAAAAA CGTAAAAAT GAGAAATGCA CACCGTAGAC CTGG |
| phwn27 | 121 bp | AGGACGTGGA ATACGGCAAG AAAACTGAAA ATCATGGAAA ATGAGAAACA TCCACTTGAC GACTTGAAA ATGACGAAAT CACTAAAAAA CGTAAAAAT GAGAGATACA CACTGAAGGC C |

[†] Chain length without space reported in sequence dataset of M. Kubista.

SET 1C A-tracts 3 (72%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|--------|---|
| phcn3 | 123 bp | ACGTGAAAAA TGAGAAATGC ACACGTGAAGG ACCTGAAATA TGGCGAGAAA ACTGAAAATC ACGGAAAATG AGAAATACAC ACTTTAGGAC GTGAAATATG GCGAGGAAAAA CTGACAAAGG CGG |
| phcn7 | 118 bp | AGAAAAACTGA AAATCACCGA AAATTAGAAA TACACACTTT AGGACGTGAA ATATGGCGAG GAAAATGGAA AAAGGTGGAA AATTTAGCAG TGTCCACTGT AGGAGGTGGA ATATGGCA |
| phcn9 | 136 bp | AGGACGTGCA ATAAGGCAAG AAAACTGAAA ATCATGGAAA ATGAGAAACA TCCACTTGAC GACTTGAAA ATGACAAAAT CACTAAAATA CGTGAAAAAT GAGAGATGCA CCCTGAAGGA CCTGGAATAT GGCAG |
| phcn11 | 124 bp | ATGGCTAGAA AACTGAAAAT CATGGAAAAA GAGAACATC CACTTGACGA CTTGAAAAT GTCGAAATCA CTAAAAAACG TGAAAATGA GAAATGCACA CTGAGGGACC TGGAATATGG CGAG |
| phcn19 | 129 bp | ATGGCGAGAA AACTGAAGTT CACGGAAAAT GGAGAAATAC ACACTTAGG ATGCAGTGAA ATATTGAGCG AAGGAAAATC GAAAAGGTG GAAAATTAG AAATGTCCAC TGTAGGACGA GGAATATGG |
| phcn28 | 122 bp | AGAAAAACTGA AAATCACCGA AAATGAGGAA TACACACTTT AGGACGTGAA ATATGGCGAG GAAAACTGAG AAAGTGGAA AATTTAGAAA TGTCCACTGT AGGATCGTGG AATATAGCAG GC |
| phcn37 | 117 bp | AGAACACTGA AAATCACCGA AAATGAGAAA TACACACTTT AGGACGTGAA ATATGGCGAG GAAAACTAAA AAAGGTGGAA AATTTAGAAA TGTCCACTGT AGGACGTGGA ATATGGC |
| phcn44 | 123 bp | ATGGCGAGAA AACTGAAAAT CACGGAAAAT GAAAATACA CACTTCAGGA CGTAAATAT GGCAGGAAA ACTGAAAAAG GTGGAAAATT TAGAAATGTC CACTGTAGGA CGTGGAAATAT GGC |
| phwn11 | 123 bp | ATGGCGAGAA AACTGCAAAT CACGGAGAAT GAGAAATACA CACTTTAGGA CGTGAAGTAT GGCAGGAAA ACTGAAAAAG GTGGAAAATT TAGAAATGTC CGCTGTAGGA CGTGGAAATAT GGC |
| phwn29 | 136 bp | AGGACGTGCA ATAAGGCAAG AAAACTGAAA ATCATGGAAA ATGAGAAACA TCCACTTGAC GACTTGAAA ATGACAAAAT CACTAAAATA CGTGAAAAAT GAGAAATGCA CCCTGAAGGA CCTGGAATAT GGCAG |
| phwn36 | 120 bp | TGGAAAATTA GAAACATCCA CTTGATGACT TGAATAATGA CGAAATCACT AAAAAACGTG AAAGATGAGA AATGCACACT GAAGGACCTG GAATATGGCG AGAAAATCTGA AAATCACCGA |

SET 2 TG/CTG RUNS (47%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|--------|--|
| phcn31 | 141 bp | GCATGCATGC ATACACGCAT GTATACGAAC ATGTACACAC ATACTCATGA ACACGCATAC ACGCGCACAT ATGCATACAT GCTTGTATAC ACACATGTAT ACGAACATGT GTACACATAC TCATAAACAC TCACACACAC C |
| phcn32 | 125 bp | TACACACACA CCACATCATG CATAACACACA CATCAATGCA ATGCATACAC ACATACATAC ACATACTAAC ACATACACTC ACACACACGC AGAAATTATG CATGCATCAT CGACATTGGC ACGCA |
| phcn33 | 133 bp | TACACACACT AACACACACA CATGCACACA TACACACAGA CACATGCACA TATAACACACA CATAACACAGC CATAACACACA CATAACACACA CATATACACA CACATGCACA CTTACACACA CATGCACACA CAC |
| phcn40 | 151 bp | AGCACTGTGA CAACACAGTG GAGCAGCTTA ACACCCACAGT GTAGCACTAT GACATCAGAG TTGAGCACTG TGTCACCACT CAGAGAACTA TGACACTACA GTAGAGCACT GTAACATCAC AGTCGAGCAC TGTAAACACCA CATATGCGCA T |
| phwn2 | 128 bp | GAGAGTAACA TAGGCACAGG TGTGGAGAGT AACACAGGC CAGGTGTGGA GAGTACACAC AGGCACAGGC GTGGAGAGTA CACACAGGC CAGGTGTGGA GAGCACACAC AGGCACAGGT GTGGAGAG |
| phwn3 | 139 bp | CACTGTGACA ACAATGTGGA ACATTGTGAC ATCACAGTGG CGAACAGTGA CGGAACAGTA AAGGAGTCTG ACAGTACAGT GGAAACAGT GACGGAACGT TGGAGCACTG TGATTACACC ATGGGACATG TTGCACCCAC |
| phwn4 | 124 bp | GAGAGTAACA CAGGCACAGG TGTGGAGAGT AACACAGGC CAGGTGTGGA AGAGTGACAC ACAGGCACAG GTGAGGAGAG TACACACAGG CACAGGTGTG GAGAGCACAC ACAGGTGCGG AGAG |
| phwn7 | 132 bp | AGCAGCAGCA GCAACAGTAG TAGAACAGC AGCACTAACG ACAGCACAGC AGTAGCAGTA ATAGAACAGCAG CAGCAGCAGC AGTAGCAGTA GCAGCAGCAG CAGCAGCAAT TTCAACAACA GCAGCAGCAG CT |
| phwn10 | 127 bp | AGACCTTGTC TCAACACACA CACACACACA CACACACACA CACACACGCG CGCACACACA CGCACACACA CATATGCACA CACACACGCA CACGCACACA CACATGCACA CGCGCACGTG CACACAC |
| phwn13 | 134 bp | CACACACACA TACTCACACA CCTGTACAC ACACACACAT GCACATATCT GCACCCACACA CAAACACATG CGTGTACACA CACATACTCA CACCTGTACC ACACACACAC ATGCACACAT CCGCACCACA CGCA |
| phwn14 | 128 bp | CTTCCTCATG CATGAGCTTG CATGAGCTTG CATATGCTCA CATAACCACAC ATGTGAGTCT ACACACAATG AGCACACACA CACACACACA CATCACTAAC CGTCTCGGTC TGGCCATCAT AGTCTGGC |
| phwn15 | 133 bp | CACACACACA CACCACATAC ACACACACAC CACATACACA CACACACACT ACATACACAC ACACACATTC ACGCACACAC ACATACACAT ACACACACAC ACCACATACA CACACATACA CACCACATAC ACA |

| | | |
|---------------------|--------|---|
| phwn16 | 140 bp | CACTGTGACA ACAATGTGGA ACATTGTGAC ATCACAGTGG CGAACAGTG CAAAGCAGCA AAGGAGTCTG ACAGCACAGT GGAAAACAGT GACAGCAGAC TGTGAGCACA GTGATTGCAC CATGGAGCAT ACTACACCCAC |
| phwn17 | 139 bp | GAGCACCTGT GACACCACAA GGGGGCCTTG TGACTGCACA GAGGGGCACT GTGTACAAC AGTGGAAATGC TGTGACAGTA CAGTGGAGCA GTGTGACAAA ACAGTGGAGT ACTGTGACAC AATAGTAGGG CAATATGAC |
| phwn18 | 128 bp | ATGCGCAGAC GCACACACAT GAGCATGCGC AGACGCACAT ACATGAGCGT ACGCAGACGC ACACACATGA GCATGCGCGC GCGACACACA CACACACACA CACACACACA CGAGTGGCAA GGCGGGGG |
| phwn20 | 122 bp | ATGCGCTGAC GCACACACAT GAGCACGCGC AGACGCACAT ACATGAGCGT ACGCAGACAC ACACACATGA GCATGCGCGC GCGACAAACAC ACACGCTCAC ACACACGAGT GGCAAGGGGG GG |
| phwn22 | 131 bp | CAATGTGACA TTACATGTAG CATGGTGAAA TCCCAGTGGG ATACTGTGAC ACCACATTGG AGCACAATGA CACCACTGTG GAGCATGTGA CACCACAGTG GAGCACTGTG AAACCTCAGT GGAGCACTGG T |
| phwn23 | 126 bp | GCAGTGCTCA CATAACAGCGC ACACATACAG TGCTCCATAT AGTGCACACA TACAGTGCAC ACATAACGGTG CTCACGTACA GTGCTCACAT ACAGTGTACA CATACAGTAC ACACATACAC TGCACA |
| phwn24 | 139 bp | CACTGTGACA ACAATGTGGA ACATTGTGAC ATCACAGTGG CGAACAGCGA CAAACAGTA AAGGAGTCTG ACAGCACAGT GGAAAACAGT GACAGAACTG TGGAGCACTG TGATTGCACC ATGGAGCATG TTACACCAC |
| phwn25 | 134 bp | ATGCGCAGAC GCACACACAT GAGCATGCGC AGGCGCACAT ACATGAGCAT ACGCAGACGC ACACACATGA GCATGCGCGC GCACACACAC ACACACACAC ACACACACAC ACACACACGA GTGGCAAGGC GGGG |
| phwn28 | 139 bp | CACTGTGACA ACAAAAGTGGG ACATTGTGAC ATCACAGTGG CGAATAGCGA CAAACAGTA ACAGGAGTCTG ACAGCACGGT GGAAAACAGT GACAGAACTG TGGAGCACTG TGGTTGCACC ATGGAGCATG TTACGCCAC |
| phwn30 | 131 bp | CAATGTGACA TCACATGTAG CATGGTGAAA TCCCAGTGGG ATACTGTGAC ACCACATTGG AGCACAGTGA CGCCACAGTG GAGCATGTGG CACCACAGTG GAGCACTGTG AAACCCACAGT GGAGCACTGG G |
| phwn32 [†] | 138 bp | TGCCAGATGA CACGTGCTAT GCCCAGGTGA CACAAGCTAT GCCCAGATGA TACGTGCTAT GCCCAGGTGA CACATGCTAT GCCCAGGTGA CACATGCTAT GCCCAAGTGA CACATGCCAT GCCAGGTGAC ACAAGCTA |

[†] Reverse complement of unlabeled file in sequence dataset of M. Kubista.

SET 3 Phased TATA (96%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|--------|--|
| phcn5 | 123 bp | AGGTCTATAA GCGTCTATAA ACGTCTATAA ACGTCTATAA GCGTCTATAA ACGCCTATAA GCGCCTATAA ACGCCTATAC GAGCCTATAA ACGCCTATAC ACGGCTATAC ACGTCTATAC ACG |
| phcn25 | 126 bp | AGGTCTCTAA GCGTCTAAAA ACGCCTATAA ACGTTTATAA ACGTCTATAA ACGCCTACAA ACGCCTATAA ACGCCTATAC AAGCCTATAA ACGCCTGTAC ACGTCTACAC ACGTCTATAC ACGTCT |
| phcn41 | 126 bp | AGGTCTATAA GCGTCTATAA GCGTCTATGA ACGTCTATAA ACGTCTATAA ACGCCTATAA ACGCCTATAA ACGCCTATAC AAGCCTATAA ACGCCTATAC ACGTCTATGC ACGACTATAC ACGTCT |
| phcn49 | 126 bp | AGGTCTATAA GCGTCTATAA ACGTCTATAA ACGTTTATAA ACGTCTATAA ACGCCTATAA ACACCTATAA ACGCCTATAC AAGCCTATAA ACGCCTATAC ACGTCTATAC ACGCCTATAC GCGTCT |

SET 4 phased TG/CA (96%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|---------------------|--------|---|
| phcn6 | 126 bp | ATTTGTAGAA CAGTGTATAT CAATGAGTTA CAATGAAAAA ACATGGAGAA TGATAAAATAC CACACTGTAG AACATATTAG ATGAGTGAGT TACGCTGAAA AACACATACG TTGGAAACCG GCATTG |
| phcn16 | 123 bp | ATTTGTAGAA CAGTGTATAT CAATGAGCTA CAATGAAAAT CATGGAAAAT GATAAAAACC ACACTGTAGA ACATATTAGA TGAGTGAGTT ACACTGAAAA ACACATCCGT TGGAAACCGG CAT |
| phcn27 | 126 bp | AACAGGATTG GTAGAACAGT GTATATCAAT GAGTTACAAT GAGAAACGTG GAAAATGATA GAAACCACAC TGTAGAACAT ATTATCTGAG TGAGTTACAC AGAAAAACAC ATTCTGTTGGA AACGGG |
| phcn48 [†] | 118 bp | ATGTAGGACA GTGTATATCA ACGAGTTACA ATGAGAAACA TGGAAAATGA TAAAAAACCAC ACTGTAGAAC AGATTAGATG AGTGAGTTAC ACTGAGAAC ACATTCTGTTG GAAACGGC |

[†] DNA-binding site for CENP-B

SET 5 No sequence (40%)

Widlund, H.R., Cao, H., Simonsson, S., Magnusson, E., Simonsson, T., Nielsen, P.E., Kahn, J.D., Crothers, D.M. & Kubista, M. (1997) Identification and characterization of genomic nucleosome-positioning sequences. *J. Mol. Biol.* 267, 807-817.

| | | |
|--------|----------------------|---|
| phcn1 | 144 bp [†] | GGCGGGTAAT TGAGCATCAG TAGGTATAGC TAAGCGGGAT GCGATACTAG CAATAGCGTC AACAAAGAGGA TAGTGGTGAG CAGAGACGTG CTGCGCGCTA CAATTGGCGT GGCAGTAATA GTCCCTGTTA GTAACCTCGGT CTTG |
| phcn15 | 145 bp [†] | CGGGAGTAGA ATGCAAGCGA GGCGGGTACG AGCTAAAGAA TGCCTGATGC AGGGATAAAC GTGAACCGTT ATACAGAAAA ATGCAGATAG AGTGAACAA GGCGAGCTTA CTGCCACGCG TTGAGAGCCA GCACCGGACA CGATA |
| phcn34 | 125 bp [†] | CAGCCCCGGC CTTGAACATAT AGAGCAGCTG AAGATAACTT TGAATTCTG ACCCTCCTAC CTCTACCTCA CGAATGTTAG GACTACAGGT GAATGCCACC ACACCCCTACT TAACACAGTG ACCAA |
| phcn35 | 145 bp [†] | GTGAGCTGTG CGGAAGCAAA AGGAAAGCGA TTAACGGTGT GCTGCATGAT AGTAAGTTAT GCCGCGGACA AGCAGCGTCG AAGCACCAGG GATGGCACAG CTGGCACTAA GGCGGGTGGT ATCAGAAGCT CCTGACAGCT TAGGG |
| phcn36 | 146 bp [†] | GGCGAAAGCG GTGAACAGTG GGTGGGAGCC CATTATATTG GTTGAGAGGG CATTGAGACC ACGCCAACAA AACATTGGTT GCATGTGATA GTTTAACCGAG CGAATGACTC GATAAGTCTT AAGATAACGG GCGTATTGGT CGTTTG |
| phcn38 | 144 bp [†] | GTGAGCTGTG CGGAAGCAAA AGGAAAGCGA TTAACGGTGT GCTGCATGAT AGTAAGTTAT GCCGCGGACA AGCAGCGTCG AAGCACCAGG ATGGCACAGC TGGCACTAAG GCCGGTGGTA TCAGAAGCTC CTGACAGCTT AGGG |
| phcn45 | 144 bp ^{†‡} | AGAGGGCGGG TGATATGGAA TCGGGGCCAA TGCGCAGTTT AAGGTTACAG ATTAGGAGTG CGCGCGGAGC TGTAAGCTCG TCGAGCGTCC ATTGGCTAGG TGGAAAGTGGAA TAGAGGCAGTC GAGGGTCCGG ACCAGGTAGC GTTG |
| phwn1 | 134 bp [†] | GC GGAGGGTG GGGCAATGGG AGCTGCGCAG CAAATACTCC GTCATCAGGG GTTAGCCGCG TGTAGCAATG GAGCTGGTAG CAGGCACGAA TGACTCGGGT TTGGGTGTAA CCTGAATAGC GGCTGTAGTC GTCG |
| phwn5 | 144 bp [*] | GAGGACAAGA GCACCTAACT ACACCAAAGC CGGACCGTTG GCGCTCACCC TGTGGTGATC AATCTCCCAC CACGCTTCC ACCTGACAGC GCAGAGTATC CCAGTCATAA TAGTTCCGCA TCAAGACAGA AACGTCAATG ACCC |
| phwn6 | 140 bp [§] | CGGGACAGTG TCGACAAGCA AAGGCGTAGG CCTACCGAGA GGCCTGGGAG CAGTGGTAAT CAGGGCAGCG GCGCGAATAG CGTACGTAGC GGGTGTCAAGC TATTACAGGC GTTACGATGC CCTATGTCGG GTGTGCGAGC |
| phwn9 | 127 bp [*] | AGGGAGGGTT CTGACCTCAG AACTCAGGAG GTGGATCAGA GCCCCAGACT GCTAGACACA TGCCCTGAAA GAGGAAAGCT TGCCTGCAGA GAGTGCTCTG ACCACTGGAA CTCAGGAAAG AGCTAGT |
| phwn19 | 137 bp [*] | TGTGAACAAAC CAATCAACGG TGGCAGTGCA GCATGGTCTA TCAGGTTGTA CAGGCCAGAG CGAGACTAAA ATCAATTCCA CACAAACCCCT CTTACCAACG TTAGGACCAT GATCTCTCGC ATCTCCCCC AACCCCCG |

| | | |
|--------|----------------------|--|
| phwn21 | 146 bp [*] | ACTCAAAGAA CAAAGATCCT GCTAACACG GCATTAGGGA ACGGGCGGTA CCGATGCCGT TCTGGTCGAC AGCGCATAGC CCCGGTCCAA CTCCGTGCGG CCTAGAACGT TACGTACCCT AGATGCAGCG GAACTCTTGC GTGTCG |
| phwn31 | 144 bp ^{\$} | CGGGCAGTAT TGCGCACGAA CAAGGTTACT TTTGAAGACCC ACATCTGTAC ATCTGGGTAG AGCAGGAAAG CAATTGGTGT GAAGTCATTG GCGTTGCTGC ACAGACCAGC GTCACAGTCG TTAGGGAGCC GGAATGCTAT CTGG |
| phwn33 | 124 bp [*] | GGGCTGTAGA ATCTGATGGA GGTGTAGGAT GGATGGACAG TATGACAAAA GGGTACTAGC CTGGGACAGC AGGATTGGTG GAAAGGTTAC AGGCAGGCC AGCAGGCTCG GACGCTGTAT AGAG |
| phwn34 | 142 bp [*] | AAGACAAAAT ATGCACGATG TCACATGCAG GACCGCCGAT TGTATTGATA CCATTACGTT ATGCGTGGAC GTCGGCTGTA GTCCTAACGCG CACCCCGACC GAGTTCTGTG TACGAAACCT ACCAGCTCCT TCGACGCGAT GT |
| phwn35 | 145 bp ^{\$} | GCGGATAACA ATTTCACATA GGAAACAGCT ATGACCATGA TTACGCAAGC GCGCAATTAA CCCTCACTAA AGGGAACAAA AGCTGGAGCT CCACGCGGTG GCGGCCGCTC TAGCCCCGGC GGATCCCAG GCTGAGGATG GGTTTAAGCA AAAGCCAGAC CAAGGACAGG AGGATGTGCA CACTGC |
| phwn37 | 136 bp [*] | TAGACCAGGT GAGCAGGAGG CGGACAGCAG GGAACAGTCT GGAGGGCAGG AAAGAGCTCT GAGGAGCCAT AGCAGGTAAA GCTGAGGATG GGTTTAAGCA AAAGCCAGAC CAAGGACAGG AGGATGTGCA CACTGC |

[†] Reverse complement of unlabeled file in sequence dataset of M. Kubista.

[‡] Chain length with extra space removed.

^{*} Sequence included in M. Kubista list of Set5 sequences and in table.

^{\$} Sequence not included in list of Set5 sequences in M. Kubista dataset (but in table).

(ii) Anti-selection sequences from the mouse genome[†]*TGGA Fragments*

Cao, H., Widlund, H. R., Simonsson, T. & Kubista, M. (1998) TGGA repeats impair nucleosome formation. *J. Mol. Biol.* 281, 253-260.

| | | |
|----|--------|--|
| 35 | 105 bp | ATCATGGTGA TGTTGATGAT GATGATGATG ATGGTGATGA TGATGATGGT GATGGCGATG ATGATGATGA TGGATGGCGA TGGTGATAAT GATATGGGA GTAGG |
| 19 | 123 bp | AGATGGATGG ATGATGGATG GATGATGGAT AGATGGATGA TGGATGGATG GATGATGATG GATGAATAGA TGGATGGATG GATGATGGAT GGATGGACGA TGGATGGATA GATGGATGGA TGG |
| 29 | 116 bp | TGGATGGATG GATGGATGGG TGGATGGATG AGATGATGGA TGGATGATAA GGTGTGATGGAT GGATGGGTGG ATGGGTGGAT GGATGGATGA GATGATGGAC GGGTGCATGA TGGATG |
| 75 | 86 bp | TGGATAGGTG GATGGGTAGA TGGATGAATG AATGAGTAGA TGGATGGATG GATGATGGAT GGATGGATGG ATGGATGGAT GGATGG |
| 44 | 119 bp | TGGATCGATG GATGGATGGG TGGATGGATC AGATGATGGA TGTGATGATA AGATCGATCG GATGGATGGG TGGATGGCCG GATGGATGGA TGAGATGACG GACGGATGGG TGATGGATG |
| 81 | 111 bp | TGGATGGATG GATGAATGGG TGGATGGATG AGATGATGGA TGGATGATAA GATGATGGAT GGATGGTGGA TGGGCGGATG GATGGATGAG ATGATGGATG GATGATGGAT G |
| 49 | 116 bp | ATAGATGGAT GAGTGGATGG ATGGATGGGT GGATGGATGG ACGGGTGGAT GGGTGGATGG GTAGATGGAT GGATGGATGA GTGGATGGAT GGATGGATGG GTGGATGGGT GGATGG |
| 62 | 115 bp | ATAGATGGAT GAGTGGATGG ATGGGTGGAT GGATAGATGG GTGGATGGGT GGATGGGTGG ATGGATGATG GATGGATGAG TGGATGGATG GATGGATGGG TGGATGGGTG GACGG |
| 57 | 112 bp | ATAGATGGAT AAGTGGATGG ATGGATGGGT GGATGGATGG ATGGGTTGAT GGGTGGATGG GTGGATGGAT GGATAAGTGG ATGGATGGAC GGATGGGTGG ATGGGTGGAT GG |
| 47 | 126 bp | TGGATCGATG GGTGGATGCG ACGGGTGGAT CGGATGAGAT GATGGATGGA TGATCAAGAT GATGATGGCA TGGGTGGATC GGGTGGATGG ATGGCATGAG ATGATCGGAT GGATGGATGA TGAATG |
| 77 | 120 bp | TGGATGGATG GATGGATGGA TGGGTGGATG GATGAGATGA TGGATGGATG ATAAGATGAT GGATGGATGG GTGGATAGGC GGATGGATGG TTGAGATGAT GGAGGGATGG ATGATAGATG |
| 23 | 117 bp | AAAGGGTGGA TGGAATGGGA TGGAATGGGG TGGAAATGGAT GGACGGATGG ATGGGTGGA TAGAATGGAT GGATGGATGG ACGAATGGAT GTGTGGATGG ATGGATGGAT GGATGGT |

| | | |
|----|--------|--|
| 80 | 109 bp | AGGTGGATGG ATGGTGGATA GATGGATGGA TGGACGGATG GATGGGTGGA TAAATGGATG GATGGATGGA CGAATGGATG TGTGGATGGA TGGATGGATG GATGGATGG |
| 86 | 119 bp | ATAGATGGAT GAGTGGGTGG ATGGATGGGT GGATGGATGG ATGGGTGGAT GGGTGGATGG CGGGATGGAT GATGGATGGA TGAGTGGATG GATGGATGGA TGGGTGGATG GGTGGATGG |

BADSECS

Cao, H., Widlund, H. R., Simonsson, T. & Kubista, M. (1998) TGGA repeats impair nucleosome formation. *J. Mol. Biol.* 281, 253-260.

| | | |
|----|--------|--|
| 24 | 93 bp | TACCAACAATG ACTTGGACAC AAGATACCCC CTCATCATCG CACCTAATTG GTATCAATCA GGGGGCCATC ACCCTCCAGA ACTAAAGTTG CTC |
| 26 | 81 bp | ATGACAGACG ACGCTGTCAA ATATGATAGC ACCAGCCGAG CTCCCCGATG TATGCCACG TTATCTTGTC CTGCTGAAGT T |
| 28 | 95 bp | AGGCTTACTC GGACATACCC CCCACTAGTC TAACTTTAAC ATTCAATGA CAAAAACCAC TGAACATTACC TAAGTGCCTG ACGTTCTTGT CGCGG |
| 48 | 117 bp | TCTAGAGTGT ACAACTATCT ACCCTGTAGG CATCAAGTCT ATTTCGGTAA TCACTGCAGT TGCATCATTT CGATACGTTG CTCTTGCTTC GCTAGCAACG GACGATCGTA CAAGCAC |
| 51 | 91 bp | AAGATCGCTA ACTATCCTGG ACTTTGCGAC GAAAATCTAG CACTAAAGGC AGGTCAACTC TTGACCACAC CTCGACGACT GCCCGCAATT A |
| 78 | 97 bp | ACGAATTACA ATAATACGCC ACATAAGAGG TATGACCCGC CCATCACTTA TCAAGTACAG CACTTGCCCTG CTATTGACTC TGTTTCTTGA GCAATCC |
| 31 | 88 bp | ACTACTTCGG TATCACAACG GCGTGAATCG CTACAAGTTA CCGGACATAA TCGTTGGTCA CTGGCAGTCC CCATATCTAC CCAAGCGT |
| 32 | 86 bp | ACCAAGATCC TGTTATCAGT CGTAACGATT AACCAACTGA CCAATAGGAA CACAGTCAGT GGGGGAATCG ATTGAGTACG GCCCTC |
| 33 | 85 bp | TTGCGCAAGT CGGCGTACTC GTGACCATT CAAGCTGTTA CCCTAGACTC TCATACCTCT TTACACTACC AATACCATAT GCGGA |
| 52 | 99 bp | ACGGTAAGGC GCACACCCGG CTTCTATCCC TCAGCACCCT CTATACCTTG CCGATATTCA CGGCAACTAC ACATCAACCA CTACGCGCTC TCCTCAGGC |
| 63 | 89 bp | CCGGCTAGCG TTTGTCCCAC TTTTCACTAC TATGCAGACC CTGATGTACC CGACTCGAGT ATCGTACCCCT CACCGGCCGT CTGGAGTTG |
| 69 | 99 bp | TACTTCGACT ACACACGCCA ATTCCGCCAA CCTCGTATCA ATTAACCTCA TGACGTGTAT ACCACCCGAC ACGCAAGGCA TCTCGCAGGC TCACCCTCG |
| 73 | 95 bp | AACGTTTCCC CGAAAGTAGG CCTGATGAGA CGACACCCTA TCTCATGTGG ACGACTCATA CGCCCTGGC ACCATTCTT CATGTAGTCA ACAGG |
| 76 | 92 bp | TTAGTCCGAA CCAGCAGACG AGTACCCCTAG CTGTCGGAGG TATCTATCAC GTGCCCCAGC TGCCACTCAT AATACTACAC GAGATCCGGC CC |
| 84 | 102 bp | AGAGGTGACA TGCGACTGAG GACATCTTAT CAGTAGTCAC AACAGCAGAT GGTGCTGCAA TGCCCAACGA TTACCGTCTG CCGCATAGCA CAAGACCGA AA |
| 85 | 99 bp | AACACGTCCC ATGTCACCCCC TGCCTGTGGG ACTCTAAAAA TGCTCACTAC GCTGAGTATA TTTTATCACA CATGTGTGGT GGACCCCCAGA ATGCTAACT |

| | | |
|----|--------|---|
| 27 | 87 bp | TACAAAATTA CGCAAGGCTA TAATGGCCCG AAGGCACGGA AGACCCGGCA AGCAACGCTA ACTGGCGCGC CAATCCTATG CTTTNNT |
| 30 | 88 bp | AACCAAAGTGA CAACTAACAC ACACAGGTGA GTTATCAGCG GGCCGGCATC CAGTTTAGGA GTGCCACGCC CATCTATGTT AGATACAA |
| 43 | 108 bp | CACCACATAG TTTGGTGAAG CCGGCTTCCA GCAAGCACAG TCGACTAACAA AAAACGAAAT ATCTGCCCG GGAGACGAGC TCCTGGATT ACCGCTCTTG CCAACATG |
| 53 | 87 bp | ATCACACAGG AAACAGCTAT GACATGGCAC ACAGAAAACA GCTATGACTG GGAAAACCCT GCCGTCGTGA CCGGGAAAAC CCTGGCG |
| 55 | 89 bp | TTATAACCAA AAAACCAGGT GAACAGAACG GCCATGCAAT AGTTCCTGCA ACAAACCTGC CTGAAATACG TACACGGAAT CTAAAGTAC |
| 56 | 77 bp | TTCACACAGG AAACAGCTAT GACTGAGAAA ACCCTGGCGT CACACAGGAA ACAGCTATGA CTGGGAAAAC CCTGGCG |
| 59 | 96 bp | TAGATTCAAG TGACGGACGC GTCTGCCGAC GCCCACTAGA CTGTGCGAAT GGTAAAAATG TTACTGAATA TCCTGGAAAG AGCACCTAGC TGCAAG |
| 66 | 101 bp | TGTGACGGTT ATGCAACTAG CACGTGATTT TCGTAAGAGGG TCACAAGATA ATACGGCGAG ATAACCTAAA CCATCGGACC CGATGACTAA CGGATACACT A |
| 67 | 84 bp | CCAGTAGGGT TTGTTCATAC TGAGTAAAAG TCTGTCCATA ACTACCTACA TGGAACGCAA TCAGTCACAG AAATTAGCGC CCGA |
| 74 | 87 bp | AAGAAAACGA TAGAGATCAA ACAGCAAACC TAGATAGTAA TACGACGGAC TCAAACCTCG GTCGGGCGAG CTGAGGTTGC ACCTAGA |

[†] Names are denoted pasHC# as the plasmid counterparts.

(iii) Synthetic SELEX sequences*

Lowary, P.T. & Widom, J., New DNA sequence rules for high affinity binding to histone octamer and sequence-directed nucleosome positioning. (1998) *J. Mol. Biol.* 276, 19-42.

| | | |
|-------|--------|--|
| 10nvp | 233 bp | GCGAGCTCTA GATA CGCTTA AAGTACTTAT CGGC GGCGTA CAAGCGTTT AGGCTCAAT TGCCTAGACC GCGGTGCCGG TAAGCTAGCG GGTCGAATGA TTGTACTTCC CCCCTCTGT CTTAACCCCC CAGCTCATCC CTCTGTATTA TTCACCCAAG GTCTCGCGCA ATTCCCCGTGA GATTGGGTAC TAATGAATCC GACCCGTGCG TGGAAGCCGA GAGGCAGATT CGT |
| 11nvp | 229 bp | ATGCACTAGA GGGTGACGAG CGCGATGCTG GGCGACACG CTGGATGTAC TGTTTCATT AGTTGTAAG GTGCCGCTG GAGGCAGCAT CACAAGTTAT AATTCTGCTCA CTTTAAGAAT GTCGCCTTCG GACTACCAGG GCGGAACCGC ACCAAGGGAC CGCTTATCTC GCCTTAACG GCCTTGCAC GCATCTAGAG TACGCTACGA CATA CGCCGA ACGTAAGCC |
| 13nvp | 233 bp | TACATAGATT GTTGTACATC TCTAGACCCG CTTAGCGTGC GCTACTGTCG ATTCTGAGCG GTTCACAACA CGGGTGCCTG GGTTCGGGCC CTCAACTGCG AGCGAGCCCC TGTTGATCCC TTGTTGGCC CTGCTCGTAC TGCTTGGCT CCATCCAAGG GGTTGAGAAC GTGGCATGCG CGAAACAGAG CCATATTAT TTCAAAGCGA TCCTCATTGCG CGTTCTGAC TAT |
| 16nvp | 233 bp | GATGCGTATT GCATACAAGG CAAGATAAAC GTCGCAGAGC TACCATATCG TGCACAGGCT GCGCAAAGTC GGGTCCCCGC GACGACGTGT CTGGTTCTC AGCTATACTG GGACTAGCCC GAGAGTACTA GAAAACCCGT TTGGAGCCTC ACGACCAAGG ACAAGAGGT AAGTGCCTAGA TTGCTGTCTA AGCCAGTTTA AGCGTACTTA GAAGGCCCTA ACCGACGGCG GAG |
| 18nvp | 232 bp | TTACAATTAA CAGTGACTTG GACACTTACT GCTACAGAAC CACAGGCAGC ATGCTTAGCC TGGCGATTGC TTGGTGCCTAA TACAACGCAC CAGGCCTGT AATCGACGTA ACTCAACGAG CCTGCCACGC TAAGCATACT TAGAACGTGC CTAACCAAGG GGTGGAGCCT ATCGGGCTGT GTGATTAAAA AATGAACTCT CTCGCTCTGG AGTCTTCCCG TACCCCTCGC TC |
| 22nvp | 231 bp | CAAGGGGGCG GGATGGGCTC TACAGCGAAC TATCACCCAT TCCGCAGCG GCACAGTTCC ATCCACTGCT GGGTGCCGG A GTGTTGCGCT TCATACGGTA ATTGCCGGGG TACTACCTGC CGAATGTGGC TTAAATGACA TGTACGCCGT GTTCCAAGGG TCTAGAGCAT CGTAGCGCCT TCCCCTGAG GAAAGTAGAC TCGAACACGG TGCATCCCTA ACCACGGCTA A |
| 24nvp | 228 bp | GACTTCGGAA CGTAAAATTCTG CTCCTGG CTTCTGCCGA CCGTCATCCC CCGTATGGAG AGCCCGGCCA CATGGTGCCTA ATAGACATGT CTTTCTACAA ATTCAAAACG GGACTACAGT TGAGCTAGGC TGACGGGGAT CTATGAAGCC CCAAGGAGTG CAGGGGTGTA CAGCTCACCG CGTACGTCAC TTTAAGCGGG TCTAGGCGTC ACTAAGGGC CGGTTGTA |
| 25nvp | 232 bp | GATCTATAGA GCTCTAGAAT ATTTATGGAG CTGAAAATCG CTCCCCCACA CCCTATACTG CCCCGTAAG AAGGTGCCGA CTATGTCTGC GGAAATTAAG AGGTATTAAA CGTGCAGCTG GAATGCTCTA GACCCCTTTA GGAGCCGCTA GAGGCCAAGG TTAGCATATT AGCTCGGTAG TTtGGCCTCA GTCAATTGGG TTCACTCCGA ACTGGACATA CCGATTGGGA AC |

| | | |
|--------------------|--------|--|
| 26nvp | 229 bp | TGGGCAAAC ATCAGTCACA AATCACTTGC TTCGCCAGA GCACGCCCG CTTCATTAA ACTGCCGGT GGTGCCTCA GTGTACGCCA GACGGACGTA GAGCCTATTG TGGAGCGTT CCACATAATC CACGAGACAG AAGATACTCA TACCAAGGGA AATCTAGTGC AAACGCAAGT GACGTAACAG TATAACCGCG CGGTGGCTAA CGACACCAAA ACTCCGATG |
| 28nvp | 226 bp | GAAGAGAAC CTTTCTCTC CCAACTAAAT GCTTAGTTGG CGTCGGTGCT ACCCCCTCAG GAAGGGTCTT AGGTGCCTCT AGACCCCTGC AGACGGCCG TTTCACTGAG TTACACTGGA TTGACGTTGT CCCACCCGGC GTTACTATCC AAGGGTCTGC CATTACGCAT TGTAGGATGT TTCAAGCTTT GACTGGGTAT TAGGAGGAAT CTCACGGTCA AACTAA |
| 29nvp | 231 bp | TGGGAGGGAC CAGTCCCGCA TGAAATTAT TAACATGAGC ACCACAATT TCCGTCCAAC ACAGGCACTC CTGGTGCCTG AATGAGGGC TAAACTGACC CTAGTTAGCT GTGTAGCGAA CTCTAGTGTG TCCTAGAGTG CCTCTCGTGC GATTCCAAGG GGTTTGGCC TGGGGATAG GCCACATAGC GGTACTATAG GAGTCTGAGC GGGCGAGTTT GCCTCTAAGA C |
| 2nvp | 232 bp | GAGTCAGCCA GCTAGAACGC TCTAGACACT GTTACGTGA CGTAGGCCAT TAGATAAGCC CCTACGGAAC GCGGTGCCGG CGTTGTAACG AGGTTGTGTT TTACACGGGA ACATTATGTC GCGTAGCGGC AATGGCGTAA CCCACCTTAC TGTTCAGG TCTCACCTCC GAGTGAATCA TCCTCCAGGG TGTGCTCCTC CGGGGTACCC CGCGATGTCC GTGGGTGCCG GA |
| 30nvp | 229 bp | TGTGCGTTGT GTAGTCACGG CGTTTGTGTC TCGATGAAAT CGGAAACCCA GAACCTAACG TGTGCTCCAC ACGGTGCCCG AAAAACGTTA GTAGGCCGGT CTACAGCGTG CTAAAGCACT CTAGAGCCGA TCGTGACCCCT GCTATGCTCT GCCAAGGGCA CCTGGTGTAC CCCTTGACG CAGGTCTGCC TCCGTGTATA CAGGACATTA CCGTGCCTG TACTATGAT |
| 34nvp | 231 bp | rTCgACGGgw gGGCCGCCTg cATGccGTTA CCTcATCTTg CtCCGCTCTA ACCACTTCAT TATCGAGCAC AGGTGCCAG ACGATTTAAT TTcCGTgGGA CGGCATcCTG CGGAAgGACG TATTCGTCG TAGCAATGGC TGTAAAGGT TCTCCAAGGA GCCTTCTAGA CCGGCTTACA GTCATCAGAA TcCAATTCTA AGcGCACCGc raATACTACT GAGGCTAggg G |
| 37nvp [#] | 229 bp | ACGAATGCAC gGGgcCCGGT CTAATGGAGG CGTAATGGAA GGCAGCTAgG AGAGAAATGC TGCATTCAGT GTCCTGGca tTttAAGctA TACTAGACGg CCGGCGCgG GACTGGAACA CTCGGATAGG CATCAGGAgT AACGCATTGCA ATAGGCACCC AGATTATTGc CCAGATTGTG CtACACCcgg gagGaGttAc GacAGTgcaA AGcacATCgG ATCTAGCtA |
| 38nvp | 230 bp | cCgGGAAGCs gcgCCAgGAt TTCCTccctT AttgGCTCTA gGTATGcTta AACgGCTtgG cgcGTTGttt GCGGTGCCCG TGTGCATGCT AGAGCctTTG GTTGAATGTG CATCAgCCTA GTATTGCAAGG AGCgccCCGt GCCAACTGTA CAcCCAAGGT ATTGCGTGTGA ACTTCgGcAC tTTTGtGcTG TCTTGAGttC gCGTTAgCgg tTTTTAGGgg tAAAtgACCA |
| 40nvp [#] | 231 bp | GcGGAAgGGT GGTggGGGTT GTTCAGGCtT CTAGTAGTGC TTAAAGTGCG TTAGAGGCC AgcGCAgcmc tCCCTGGCA CgGGtccCCc cACTGAATAG TaCCTATcct ATTGTTcGccG TtttacCGAG GGgtTTaGGA GGcCATACAA AAtGGCACCG TTAAGAtccG ccaggAGGcA CGcCGTgGAt cGaGatCTgg CtgcgACatA aTgcCATgAt TCctgAcCaT t |

| | | |
|-----------------------------|--------|---|
| 41nvp [#] | 230 bp | AGCTGGAAAG TGTAATAGGG CGGGCGCGGG GCGGACACTA TTCgAAggCT gTGTGcATCA TAGTCTGGCA CCTTGGCAGA ATGAGGAGAT ATTGCgCCCT GTACCGGAAA ACgGCTCAGA AcGACGTAAC AGamgccCTA AGcgCACCTA gGGGCACCTA tCTCGTTCGA ACGGGTGTC CACGCgGTTTC TGcgAATCCT gAACCGGGGA TAGCAGTAGG TgACggCACT |
| 52nvp | 232 bp | GGACCCGtTA TtgGAATTGA GTCGTATGTC CGACgGCGCG TTGAAGTGGC CGAtTTTCA ACTACACgGC ATGGTGCCCC CCTCCATAGT CGTGATCTGA ATTccCGCGGC TACATGCGct GTGTCTTCTA GACCCTCTAG GAGCACGTTA GAgGCCAAGG CAAGCACGGt cCCGGTAACG AACgGGGTTG CACtGGTACG CacCCCTAGA TgGGcAGCTT GGAACGcCTA CT |
| 54nvp | 230 bp | AGAACCTTCT ACATACGCTT AGGGTGAcGc ACTCCTcAtT TCTGAGCCTC GtGCtTTAagg gCGTATAAgG AAGGTGCCAG TCTCGTAGTG TTATAAGCGc GCCCGACGTT GTCAAACGGG CGGCATCTC TCTTGGCCGT GGTGTTTATT TGCCAAGGT TGCGTGCCTA CCATGAAAGTC TTTTATTGA CTCACCCAAAC GAACACACTA GTGCGTACCT cCCGCTTACg |
| 5nvp | 231 bp | GGCTAACTAG GCATCATTAG GTTGTGTGTT TTAGGCCTCT CCCAGCGTCT AACAGTGCTT AGCCACACCG CTGGTGCCAG TGCAcGACTT TACGATAACAA TGCGGATGCT TATGGCGAAT TCCCTACTGG AGATCCCTCA CTACTTGCG TTGCCCAAGG CGTACTGAGG GTATCGACAG CACCACGTA AATTTTCCAG TGGGGACTCA GGAGTCTTTG CGAAAGACTA G |
| 602nvp_rev_rev [#] | 232 bp | GGCAAGGTGCG CTGTTCAATA CATGCACAGG GTGTaTGTAT CCGACaCGtG CCTGGAGACT AgGAAGTAAT cCCCTGGCG GTTaAAATGC gGGGGACAGC gCGTACGTgc GTTTAAGCGG TGCTAGAGCT gtCTAcGACC AATTGAGCGG CCTCGGCACC gGGATTCTcC AGGACGGCG CGTATAGGGT cCATCACATA agGGATGAAC TCGGTGTGAA GAATCATGCT TT |
| 603nvp | 234 bp | CGagacATAC ACGaATatgG CgTTTCCTA GTACAAatCA CCCCAGCGTG AcgCGTAAaa TAATCGACAC TCTCGGGTGC CCAGTTCGCG CGCCCaCTA CCGTGTGAAG TCGTCACTCG GGCTTcTAAG TACgcTTAGg cCACggTAGA ggcaatCCA AGGCTAACCA CGTGCATCG ATGTTGaAAG AGGcCCTccG TCctTATTAC TTCaAGTccc TGGGgtACCG TTtc |
| 604rnvp | 233 bp | GTCGTCTGCA CAAATACGGA ACCTTTGGty CggTTTGCT CTAAGACACG GGCgGCACtC TAACTAGGCT TAAGGTGCCG TAAAGCCGAT TCTGAGTATA AtcCTGTCTC TTGACTTGtC TCAGGGCTAA GTTGACTcGA TGtCGTGACA TCACCCCAAG GCGATCTTGT TTGTAGTcCC CCGTsTATCG TGGGGCCGCG AGACATAGCA kCCAATAGGC ATGATGAATA GTC |
| 605nvp | 231 bp | TACTGGTTGG TGTGACAGAT GCTCTAGATG GCGATasmGA CAGGTCAAGG TTCGGGAcac GCGGGATATg GGGTGCCTAT cGCACATTGA GTgcgaGACC GGTCTAGATA CGCTTAAACG AcGTTACAAC CCTAGccccG TCGTTTTAGC CGCCAAGGG TATTCAAGCt CGACGCTAAT CACCTATTGA GCCGGTATCC ACCgTcACGA CCATATTAAT AgGACACGcC G |
| 607nvp_rev_rev | 227 bp | CTTTGGCGGA GAATGCGTAG GTGAGTGtt tgGAgACGgg aAgGCATaaA ACACCcgGAG CCTAACGAGC GCCTTGGtAt cCGGaacggg tTCTAGTACC cGTTAGCgTG gTTTAGAGGG gCAAAGAAC ATCTttcccC CCCCCGAGATA CgGGCACCGt TCgGAcCCTg GTTAGTcCAG TGCTACTGCC GGTTCCCTAGC CTAAGGCAG GATGcCTATT AGaAAGG |

| | | |
|-----------------------------|--------|---|
| 609nvp | 230 bp | TAATCTTAGC CGGTGTGCAT TACAAGCACT ACAGTGACGG ATGATCTCTA TGCGGATCTT TcAATCATGC GGGTGCCGAG TAGcGTgCcG caGTTGATGG TTCAgCCGAC GAAGCAGGCg GAACCCACTC CTAACGATGC CCACACTAT CCTCCAAGGG GCTCTATAcC CCTTTAAAgT GctGCGCTGG GCATTGGCTC CgTTTCCCC TGTCTTCCAC CGTGCAGTAA |
| 611nvp ^{#†} | 232 bp | GaACGCaAAT CTCAGATgGT gAGTAgGGGG CAGTTGA _g GG GCTTGGTCTG TGTTAACGC GCTTcTTCAg GGCCTGGAG CTCTCTCTTG AGCTTGCTGA GCAAtcgTCG ACATTAGcT TCTGCGTGA _g CGGCGTCATT AGTGAGAATG CCAAGGCACC GGCATTGCGC gTGAgATGGG CTAGGCa _a CG cgCTAAAGcgt ATCTaGAACg CGCTACGAAA CATACGCatG TT |
| 613nvp | 232 bp | TAACTAGCAT GGACCCGATT GTACGCCGTA ACACTCGCGC TCGGTGTACC TTAGTcCTAG TATAGGC _{GT} A TTGGTGC _{CA} A TTGCGC _{cg} AG CgTTGtaGCC GtGGag _t Gtc GttGtCGtAT GGGGGCTCTA GATGTGCTTA AACGGGTGGG TsGccCAAGG CcTGCATTAT TGCGGAGTAT GGCCACGcTT CCGTGCCGCT CCcTAGTCcG ACCcTtcACA CTCTCACTCG CG |
| 615fnvp | 229 bp | ACACTTGTAC AACAGGACGC CGTTATCTTC CCCTCCAGTC GGGACGGCT CTCCAACC _a T GCCAAGCGAG CGGTGCCAGC AAGGATT _{CG} G TCTCTACGTG CATCTAAGAC CCCTTAGAGT GCTCTAcTCG CTCTcGCTAG CTcCGCGAGA ACCAAGGCG GATTaATTGG CACGGGAGGT TTCTACaaCC GCACTACGTC TGCTGACGTT CGAgCCCCCT CAAACATGt |
| 618nvp_rev_rev | 232 bp | CgGACTAAAC GAACGCGtTc GtTTACAT _{TG} TGCgaAgGGG AtTGGCGTT _C TACGACAAatt tCtgGGAACA GCCCTGGTG GCTCTAGGgA GCTCTAGATG AGCTTAGC _g G TCTGTAGAC _g CAATTCTGGG cATTTCGCT CGTCTGGAtC tGTAGGCACC tGCTCGGTCA gGTACaACtT TgaAAAGGCG cCAGTTATGA G _C c _g GTATCG TgGGCTTTgG GTAgcccAcc CC |
| 620nvp_rev_rev [‡] | 231 bp | GggACCCAGC GTGCCcAGCG gTCTCTAGaT AcgcttaAAG TACTCTACGC ACTAAAaGAG GcAGCTTG _{gc} CGGGTGCCGC GcAGTGTAAA GTGgATACgc tGGGccTGAC GTATCCGAGG ACgCTCGC _g T GTCACTcTTT GCCTTCGCC CCCCCAAGGA GAAGCCTGAT ACAAAacCCAT TCTGCCCGCG AGTCAGTCCG GTCA _G TGA TACGGCGACC GgtAGATCTT C |
| 621rnvp | 232 bp | TACAGGGCGG TTCCCTAGCT GTTGcATAAA GGCGGTGGT TCGTCGCC _{CC} CCCTAAAGA TAATCCTGCG TAGGTGCCCG TGGAGCCGTT CTATTGACCC TTTACGATCG TTTAAAGGGG TCTAGAGCTA GCTAGCTTGT TcAGTCTAGC CCCACCAAGG ACTgGTgGCG TATCAGTTCA CGgcCTCC _{cg} GGTgGT _C GG TACTT _{Ag} GA ATATCC _{cg} T TACATCCGAC AT |
| 624bnvp [#] | 231 bp | ACTCTAGCAA CTGGTgCG _g C GACTcGG _g A CGATTAGGTT GCAATCCTAG ACACCCATCC AGAtTGCACT GTCCTGG _{Ac} CCAGAGCCC _g CgGAgGgACC GATTCTAGT TTcCTAGTCT CTGGGTA _{Ac} C GAAGC _{CC} CAT ACGGAAACGA GCCAGGCACC GTGCAAACG TcCAGAGTGA gCTGTcCTAT CGTTTAAGCG GTCCTAGAGC CTTCTAAGCT TGCAACCACAA |
| 626nvp | 230 bp | xxxxxGGwGG GAATTTGwG ATwGTTAwGC TCCACCAwGC CTTGTCGCTC TgCtTCGATG AGAGTCGACC GGTGCCgGGT AtTGtATCGC CGCTTGACTC TGGAAATgGCG TCTACGTAGC gCTAAGCACT ATTAGAGTCC TCTCCtGCAT CTCCAAGGAT AGtGCCTATA AATCGTCCAC CTGTgGCATT ATcCGGTGCC CTTTC _g G _g AC gTGCTTTTA GTGTC _g GGTG |

| | | |
|---------------------|--------|---|
| 628fnvp_rev_rev | 232 bp | TGCGGTTGGG CTAATCGGGG GCTTGGCGCG TAAACCTACC GTTCCGACAC CTGTTCAAAG TTTCTGACCA GTGGTGCCTG GTCTCTGAAC TGCTGTAGAG AGGCCTAGAC gTGCTTAGCG TGCAGTAGAA CCGATTCTAA ACCGTTTGAG GACGCCAAGG GTTAATGCGC ATAGgccgTT GCATGGCCCC TTGcTCAAGC CGGCTGCCAA CCAGGGccAG AGTCTCCGTT TG |
| 69nvp | 231 bp | TCgCATCcac CCTGTgAAGT gGAGGGTCGA CGTTAA ^t TTA CCATaccCCG cATAAACACGT cACGGCTAAC AGGTGCCAA ^t CTCCTCGGAA AGAATATCAG GatCGcg ^t TA cCGCACgGGG GGAGCTCTAG AGTGGcTTAA ACGACCGCAG acGCCAAGGG GAACAGGCTG cAGGAGGTgG CCGgGACtCt tcctgCgATC GAACGctCtC ttGTAGAATT GGATcCTCgG A |
| 6nvp | 232 bp | TGGACACTTT TATGTGTTA CTCGACCTTC CTCAAACCTc GCCTTGGGCT GACTCGAATT TTCCAGGCTG CAGGTGCCGG TGGAGCCTCT AGGTGTGCTC AGAGGACGGT AGAGCCCAGA TCTAGTGCTC TCCC GGTTAT TATGTCGCCT TCCCCCAAGG GACGGCGCAA GTTCCACACG AGCAACGCAG ATCTGGGTCC TGATCACTCG AAAGCCGTCG CTTCCCATAG AC |
| 73nvp | 230 bp | GAGAGAGCTG ATAGGCacGC ggacTCACgt GGGTCCCT ^t TACGGTGGTG GCAGGGAGGGC TAGGATGATT GTAGGTGCCT CTAAGTGTGC TTAAAACG ^a T cCACGGACcG CTcCTGTCgG TTTCTACACG tGTCGGACTT AATCAAAGCT CACTACCAAG GGCgGCgACG TAGccgaTAT CCGCaAAACT ACCATgaGTG GgCAgCctCc GcGcGaCtcc gGGATCTgGA |
| 7nvp | 233 bp | GCACCTGCGT CCCAGCCTTC TCCAGATGAG TTTCCACAGT GTCCCTCAGT TTCACGCTTA AAATGCTGCT TTCCGGTGCCT CTGCGTGT ^{TTT} AGGCACTACT AGAGCATTCC ACGGCTTCT TTTACACTTG ATGGTCTACG CTCTTACGTT CCATGCCAAG GACTGAGGCC TAGCACGATC TAGCcTCTCC CGTGCCTGCCG GGAAAATACG CGTCCATCGT TGCTCTTCC TCT |
| 83nvp ^{#§} | 228 bp | ATGCGGATAc AGCAACGGAT GGATCGGgAC AGCCAATCGG TGCCTCCCGT GGGAGTAAAT CGACAGGCAT ACCCTGGAG CCCGCGTCTA CCCGGTGCTC TGAAAACggcC CCAAATGCC TGTAAGGCAT CCTAACGATA CTCCTGCGAT aCTAGGCACC TATGGAAGAT TGGAGTGGGT GTCGGACAGT TCATTAGCG CAacGGGAGA CCCGgcCGC ^t waGCCCTA |

* Single and double underlined sequences are restriction fragment sequences used to ligate segments extracted in selection experiments.

[#] Reverse complement of restriction fragments.

[†] Restriction fragment sequences overlap with reverse complements.

[§] Chain contains second restriction fragment.

[‡] Sequence of reverse complement is identical to original sequence.

(iv) High-resolution positioning sequences[†]

Crystallographic DNA sequence

Davey, C.A., Sargent, D.F., Luger, K., Mäder, A.W. & Richmond, T.J. (2002) Solvent mediated interactions in the structure of the nucleosome core particle at 1.9 Å resolution. *J. Mol. Biol.* **319**, 1087-1113.

| | | |
|--------|--------|---|
| pd0285 | 146 bp | ATCAATATCC ACCTGCAGAT TCTACCAAAA GTGTATTTGG AAACTGCTCC ATCAAAAGGC ATGTTCAGCT GAATTCACT GAAACATGCCT TTTGATGGAG CAGTTCCAAT ATACACTTTT GGTAGAATCT GCAGGTGGAT ATTGAT |
| pd0286 | 146 bp | ATCTCCAAAT ATCCCCTGCG GATCGTAGAA AAAGTGTGTC AAACTGCGCT ATCAAAAGGA AACTTCAACT GAATTCACT GAAAGTTCCC TTTGATAGCG CAGTTGACA CACTTTTCT ACGATCCGCA AGGGATATTT GGAGAT |
| pd0287 | 147 bp | ATCAATATCC ACCTGCAGAT ACTACCAAAA GTGTATTTGG AAACTGCTCC ATCAAAAGGC ATGTTCAGCT GGAATCCAGC TGAACATGCC TTTTGATGGAG GCAGTTCCA AATAACACTTT TGGTAGTATC TGCAAGGTGGA TATTGAT |

Bao, Y., White, C.L. & Luger, K. (2006) Nucleosome core particles containing a poly(dA·dT) sequence element exhibit a locally distorted DNA structure. *J. Mol. Biol.* **361**, 617-624.

| | | |
|--------|--------|---|
| pd0755 | 147 bp | ATCAATATCC ACCTGCACAT TCTACCAAAA GTGTCAAAAA AAAAAAAA ATCATGATAA GCTAATTTGG CTGACTCAGC TGAACATGCC TTTTGATGGAG GCAGTTCCA AATAACACTTT TGGTAGTATC TGCAAGGTGGA TATTGAT |
|--------|--------|---|

TG-pentamer

Shrader, T. E. & Crothers, D. M. (1989) Artificial nucleosome positioning sequences. *Proc. Natl. Acad. Sci., USA* **86**, 7418-7422.

| | | |
|-------------|--------|---|
| TG-pentamer | 190 bp | TCGGTGTAG AGCCTGTAAC TCGGTGTAG AGCCTGTAAC TCGGTGTAG AGCCTGTAAC TCGGTGTAG AGCCTGAAC TCGGTGTAGA GCCTGAAC GGTGTAGAG CCTGAACCTCG GTGTAGAGC CTGAACCTCGG TGTTAGAGC TGAACTCGGT GTTAGAGCCT GAACTCGGTG TTAGAGCCTG |
|-------------|--------|---|

pGUB

An, W., Leuba, S.H., van Holde, K. & Zlatanova, J. (1998) Linker histone protects linker DNA on only one side of the core particle and in a sequence-dependent manner. *Proc. Natl. Acad. Sci., USA* **95**, 3396-3401.

Kassabov, S.R., N.M. Henry, M. Zofall, T. Tsukiyama & Bartholomew, B. (2002) High-resolution mapping of changes in histone-DNA contacts of nucleosomes remodeled by ISW2. *Mol. Cell. Biol.* **22**, 7524-7534.

| | | |
|------|--------|---|
| pGUB | 183 bp | GATCCTCTAG ACGGAGGACA GTCCTCCGGT TACCTTCGAA CCACGTGGCC GTCTAGATGC TGACTCATGG TCGACACGCG TAGATCTGCT AGCATCGATC CATGGACTAG TCTCGAGTTT AAAGATATCC AGCTGCCCGG GAGGCCTTCG CGAAATATTG GTACCCCCATG GAATCGAGGG ATC |
|------|--------|---|

Table S3. Properties of DNA base-pair steps used in knowledge-based potentials**(i) Number of base-pair steps included in derived ‘energy’ functions[†]**

| Step | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|----------------------------------|--------|------|------|---------|------|
| CG | 88 | 160 | 160 | 118 | 160 | 118 |
| CA | 110 | 177 | 166 | 143 | 166 | 143 |
| TA | 134 | 236 | 232 | 212 | 238 | 218 |
| AG | 106 | 168 | 157 | 133 | 157 | 133 |
| GG | 97 | 146 | 139 | 95 | 139 | 95 |
| AA | 129 | 169 | 169 | 166 | 181 | 178 |
| GA | 117 | 175 | 173 | 146 | 173 | 146 |
| AT | 140 | 236 | 230 | 202 | 234 | 202 |
| AC | 137 | 189 | 188 | 168 | 188 | 168 |
| GC | 86 | 182 | 164 | 140 | 164 | 140 |
| Generic | 1840 | 2862 | 2770 | 2374 | 2798 | 2402 |

[†]Counts exclude terminal dimer units and steps with single-stranded nicks and mismatches within the selected sets of high-resolution structures.

(ii) Average values and dispersion of Tilt, $\langle \theta_1 \rangle \pm (\sigma_{\theta_1})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|----------------------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| CG | 0.0 _(4.2) | 0.0 _(3.9) | 0.0 _(3.9) | 0.0 _(3.2) | 0.0 _(3.9) | 0.0 _(3.2) |
| CA | 0.5 _(3.7) | 0.1 _(3.1) | 0.2 _(3.2) | -0.3 _(3.2) | 0.2 _(3.2) | -0.3 _(3.2) |
| TA | 0.0 _(2.7) | 0.0 _(2.7) | 0.0 _(2.7) | 0.0 _(2.8) | 0.0 _(2.7) | 0.0 _(2.8) |
| AG | -1.7 _(3.3) | -1.1 _(2.5) | -1.0 _(2.5) | -1.0 _(2.5) | -1.0 _(2.5) | -1.0 _(2.5) |
| GG | -0.1 _(3.7) | 0.7 _(3.6) | 0.6 _(3.5) | 0.4 _(3.6) | 0.6 _(3.5) | 0.4 _(3.6) |
| AA | -1.4 _(3.3) | -1.1 _(2.5) | -1.1 _(2.5) | -1.1 _(2.5) | -0.9 _(2.6) | -0.9 _(2.6) |
| GA | -1.5 _(3.8) | -1.5 _(2.8) | -1.6 _(2.8) | -1.4 _(2.8) | -1.6 _(2.8) | -1.4 _(2.8) |
| AT | 0.0 _(2.5) | 0.0 _(2.4) | 0.0 _(2.5) | 0.0 _(2.3) | 0.0 _(2.4) | 0.0 _(2.3) |
| AC | -0.1 _(3.1) | 0.6 _(2.9) | 0.6 _(2.9) | 0.7 _(2.9) | 0.6 _(2.9) | 0.7 _(2.9) |
| GC | 0.0 _(3.9) | 0.0 _(3.6) | 0.0 _(3.8) | 0.0 _(3.9) | 0.0 _(3.8) | 0.0 _(3.9) |
| Generic | 0.0 _(3.6) | 0.0 _(3.1) |

(iii) Average values and dispersion of Roll, $\langle \theta_2 \rangle \pm (\sigma_{\theta_2})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|-----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| CG | 5.4 _(5.2) | 5.5 _(5.7) | 5.5 _(5.7) | 6.0 _(5.8) | 5.5 _(5.7) | 6.0 _(5.8) |
| CA | 4.7 _(5.1) | 5.1 _(5.0) | 5.2 _(4.9) | 4.9 _(4.9) | 5.2 _(4.9) | 4.9 _(4.9) |
| TA | 3.3 _(6.6) | 2.5 _(5.8) | 2.4 _(5.8) | 2.6 _(5.7) | 2.7 _(6.1) | 3.0 _(6.0) |
| AG | 4.5 _(3.4) | 4.1 _(3.7) | 4.2 _(3.5) | 4.2 _(3.4) | 4.2 _(3.5) | 4.2 _(3.4) |
| GG | 3.6 _(4.5) | 5.0 _(4.6) | 4.8 _(4.6) | 5.0 _(4.7) | 4.8 _(4.6) | 5.0 _(4.7) |
| AA | 0.7 _(5.4) | 0.7 _(4.5) | 0.7 _(4.5) | 0.7 _(4.5) | 1.7 _(5.7) | 1.7 _(5.7) |
| GA | 1.9 _(5.3) | 1.9 _(5.4) | 1.8 _(5.4) | 2.6 _(3.9) | 1.8 _(5.4) | 2.6 _(3.9) |
| AT | 1.1 _(4.9) | 1.0 _(3.7) | 1.0 _(3.6) | 0.9 _(3.7) | 1.0 _(3.6) | 0.9 _(3.7) |
| AC | 0.7 _(3.9) | 1.6 _(3.3) | 1.5 _(3.3) | 1.5 _(3.4) | 1.5 _(3.3) | 1.5 _(3.4) |
| GC | 0.3 _(4.6) | 1.2 _(4.6) | 0.4 _(4.0) | 0.7 _(3.7) | 0.4 _(4.0) | 0.7 _(3.7) |
| Generic | 2.7 _(5.2) | 2.9 _(4.9) | 2.9 _(4.9) | 3.0 _(4.7) | 3.0 _(5.0) | 3.1 _(4.8) |

(iv) Average values and dispersion of Twist, $\langle \theta_3 \rangle \pm (\sigma_{\theta_3})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| CG | 36.1 _(5.5) | 34.4 _(3.7) | 34.4 _(3.7) | 33.9 _(3.7) | 34.4 _(3.7) | 33.9 _(3.7) |
| CA | 37.3 _(6.5) | 35.0 _(4.9) | 35.5 _(4.6) | 35.8 _(4.6) | 35.5 _(4.6) | 35.8 _(4.6) |
| TA | 37.8 _(5.5) | 37.4 _(7.3) | 37.5 _(7.3) | 37.6 _(7.5) | 37.1 _(7.7) | 37.1 _(7.9) |
| AG | 31.9 _(4.5) | 32.5 _(4.6) | 32.6 _(4.6) | 32.3 _(4.5) | 32.6 _(4.6) | 32.3 _(4.5) |
| GG | 32.9 _(5.2) | 33.3 _(4.5) | 33.4 _(4.5) | 32.7 _(3.9) | 33.4 _(4.5) | 32.7 _(3.9) |
| AA | 35.1 _(3.9) | 35.1 _(3.9) | 35.1 _(3.9) | 35.1 _(3.9) | 34.3 _(4.8) | 34.3 _(4.8) |
| GA | 36.3 _(4.4) | 35.5 _(4.2) | 35.7 _(4.1) | 35.5 _(4.2) | 35.7 _(4.1) | 35.5 _(4.2) |
| AT | 29.3 _(4.5) | 29.8 _(4.0) | 29.8 _(4.0) | 29.8 _(4.2) | 29.5 _(4.4) | 29.8 _(4.2) |
| AC | 31.5 _(4.2) | 31.7 _(3.7) | 31.7 _(3.7) | 31.5 _(3.6) | 31.7 _(3.7) | 31.5 _(3.6) |
| GC | 33.6 _(4.7) | 33.7 _(5.0) | 34.3 _(4.6) | 33.5 _(4.4) | 34.3 _(4.6) | 33.5 _(4.4) |
| Generic | 34.2 _(5.5) | 33.8 _(4.9) | 34.0 _(4.9) | 33.8 _(4.8) | 33.8 _(5.0) | 33.6 _(4.9) |

(v) Average values and dispersion of Shift, $\langle \theta_4 \rangle \pm (\sigma_{\theta_4})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| CG | 0.00 _(0.87) | 0.00 _(0.79) | 0.00 _(0.79) | 0.00 _(0.75) | 0.00 _(0.79) | 0.00 _(0.75) |
| CA | 0.09 _(0.55) | -0.05 _(0.67) | -0.08 _(0.67) | -0.15 _(0.67) | -0.08 _(0.67) | -0.15 _(0.67) |
| TA | 0.00 _(0.52) | 0.00 _(0.58) | 0.00 _(0.58) | 0.00 _(0.55) | 0.00 _(0.58) | 0.00 _(0.54) |
| AG | 0.09 _(0.69) | 0.19 _(0.64) | 0.20 _(0.65) | 0.20 _(0.65) | 0.20 _(0.65) | 0.20 _(0.65) |
| GG | 0.05 _(0.76) | 0.02 _(0.67) | 0.01 _(0.68) | 0.02 _(0.73) | 0.01 _(0.68) | 0.02 _(0.73) |
| AA | -0.03 _(0.57) | 0.08 _(0.35) | 0.08 _(0.35) | 0.08 _(0.35) | 0.10 _(0.35) | 0.10 _(0.35) |
| GA | -0.28 _(0.46) | -0.21 _(0.49) | -0.22 _(0.49) | -0.21 _(0.50) | -0.22 _(0.49) | -0.21 _(0.50) |
| AT | 0.00 _(0.57) | 0.00 _(0.54) | 0.00 _(0.54) | 0.00 _(0.55) | 0.00 _(0.55) | 0.00 _(0.55) |
| AC | 0.13 _(0.59) | 0.22 _(0.55) | 0.22 _(0.55) | 0.21 _(0.57) | 0.22 _(0.55) | 0.21 _(0.57) |
| GC | 0.00 _(0.61) | 0.00 _(0.70) | 0.00 _(0.72) | 0.00 _(0.74) | 0.00 _(0.72) | 0.00 _(0.74) |
| Generic | 0.00 _(0.64) | 0.00 _(0.61) | 0.00 _(0.61) | 0.00 _(0.62) | 0.00 _(0.61) | 0.00 _(0.62) |

(vi) Average values and dispersion of Slide, $\langle \theta_5 \rangle \pm (\sigma_{\theta_5})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|-------------------------|
| CG | 0.41 _(0.56) | 0.36 _(0.57) | 0.36 _(0.57) | 0.55 _(0.40) | 0.36 _(0.57) | 0.55 _(0.40) |
| CA | 0.53 _(0.89) | 0.22 _(0.91) | 0.33 _(0.81) | 0.50 _(0.75) | 0.33 _(0.81) | 0.50 _(0.75) |
| TA | 0.05 _(0.71) | 0.37 _(0.93) | 0.39 _(0.92) | 0.46 _(0.93) | 0.43 _(0.95) | 0.50 _(0.95) |
| AG | -0.25 _(0.41) | -0.32 _(0.45) | -0.27 _(0.41) | -0.22 _(0.40) | -0.27 _(0.41) | -0.22 _(0.40) |
| GG | -0.22 _(0.64) | -0.52 _(0.62) | -0.45 _(0.54) | -0.27 _(0.50) | -0.45 _(0.54) | -0.27 _(0.50) |
| AA | -0.08 _(0.45) | -0.16 _(0.33) | -0.16 _(0.33) | -0.15 _(0.33) | -0.11 _(0.38) | -0.11 _(0.38) |
| GA | 0.09 _(0.70) | -0.12 _(0.53) | -0.10 _(0.51) | -0.02 _(0.48) | -0.10 _(0.51) | -0.02 _(0.48) |
| AT | -0.59 _(0.31) | -0.66 _(0.33) | -0.64 _(0.32) | -0.58 _(0.28) | -0.64 _(0.32) | -0.58 _(0.28) |
| AC | -0.58 _(0.41) | -0.63 _(0.32) | -0.62 _(0.32) | -0.58 _(0.37) | -0.62 _(0.32) | -0.58 _(0.37) |
| GC | -0.38 _(0.56) | -0.33 _(0.55) | -0.21 _(0.41) | -0.15 _(0.39) | -0.21 _(0.41) | -0.15 _(0.39) |
| Generic | -0.09 _(0.69) | -0.21 _(0.67) | -0.17 _(0.64) | -0.07 _(0.63) | -0.16 _(0.65) | -0.07 _(0.64) |

(vii) Average values and dispersion of Rise, $\langle \theta_6 \rangle \pm (\sigma_{\theta_6})$, in protein-bound DNA dimers

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| CG | 3.39 _(0.27) | 3.41 _(0.22) | 3.41 _(0.22) | 3.38 _(0.23) | 3.41 _(0.22) | 3.38 _(0.23) |
| CA | 3.33 _(0.26) | 3.38 _(0.26) | 3.37 _(0.23) | 3.35 _(0.22) | 3.37 _(0.23) | 3.35 _(0.22) |
| TA | 3.42 _(0.24) | 3.32 _(0.21) | 3.33 _(0.21) | 3.30 _(0.19) | 3.33 _(0.21) | 3.31 _(0.19) |
| AG | 3.34 _(0.23) | 3.35 _(0.23) |
| GG | 3.42 _(0.24) | 3.45 _(0.24) | 3.45 _(0.24) | 3.38 _(0.20) | 3.45 _(0.24) | 3.38 _(0.20) |
| AA | 3.27 _(0.22) | 3.25 _(0.17) | 3.25 _(0.17) | 3.25 _(0.16) | 3.26 _(0.17) | 3.25 _(0.16) |
| GA | 3.37 _(0.26) | 3.32 _(0.20) | 3.32 _(0.21) | 3.27 _(0.17) | 3.32 _(0.21) | 3.27 _(0.17) |
| AT | 3.31 _(0.21) | 3.24 _(0.17) | 3.24 _(0.17) | 3.24 _(0.17) | 3.24 _(0.16) | 3.24 _(0.17) |
| AC | 3.36 _(0.23) | 3.27 _(0.20) | 3.27 _(0.20) | 3.27 _(0.21) | 3.27 _(0.20) | 3.27 _(0.21) |
| GC | 3.40 _(0.24) | 3.36 _(0.24) | 3.33 _(0.24) | 3.29 _(0.22) | 3.33 _(0.24) | 3.29 _(0.22) |
| Generic | 3.36 _(0.25) | 3.34 _(0.23) | 3.33 _(0.22) | 3.31 _(0.21) | 3.33 _(0.22) | 3.31 _(0.21) |

(viii) Relative base-pair flexibility V of protein-bound DNA dimers[†]

| Step | Olson <i>et al.</i> * | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------|-----------------------|--------|------|-----|---------|------|
| CG | 12.1 | 4.9 | 4.9 | 2.3 | 4.9 | 2.3 |
| CA | 9.8 | 7.1 | 5.1 | 4.7 | 5.1 | 4.7 |
| TA | 6.3 | 7.6 | 7.5 | 6.1 | 8.4 | 6.8 |
| AG | 2.1 | 1.6 | 1.3 | 1.1 | 1.3 | 1.1 |
| GG | 6.1 | 4.1 | 3.6 | 2.6 | 3.6 | 2.6 |
| AA | 2.9 | 0.6 | 0.6 | 0.6 | 0.8 | 0.8 |
| GA | 4.5 | 1.9 | 1.8 | 1.0 | 1.8 | 1.0 |
| AT | 1.6 | 0.9 | 0.8 | 0.7 | 0.9 | 0.7 |
| AC | 2.3 | 0.9 | 0.9 | 1.1 | 0.9 | 1.1 |
| GC | 4.0 | 3.5 | 2.2 | 1.8 | 2.2 | 1.8 |
| Generic | 9.2 | 5.2 | 4.8 | 4.2 | 5.1 | 4.5 |

[†]Deformability values, in units of $(\text{\AA}^\circ)^3$ given by the products of the eigenvalues of the covariance matrix of the averages and products of the six step parameters.

*W.K. Olson, A.A. Gorin, X.-J. Lu, L.M. Hock & V.B. Zhurkin (1998) DNA sequence-dependent deformability deduced from protein-DNA crystal complexes, *Proc. Natl. Acad. Sci., USA* **95**, 11163-11168.

Table S4. Comparative ‘cost’ of nucleosomal deformation of individual base-pair steps with knowledge-based functions based on different subsets of observed protein-bound DNA conformations[†]

(i) Pyrimidine-purine (YR) base-pair steps

| <i>CG</i> | | | | | | |
|---------------------|----------------------------------|--------|------|------|---------|------|
| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
| $\langle E \rangle$ | 7.4 | 4.5 | 4.5 | 6.4 | 4.5 | 6.4 |
| E_0 | 0.8 | 0.4 | 0.4 | 0.7 | 0.4 | 0.7 |
| E^{\dagger} | 24.8 | 13.0 | 13.0 | 18.8 | 13.0 | 18.8 |
| SH_0 | -2.4 | -2.4 | -2.4 | -2.4 | -2.4 | -2.4 |
| SH^{\dagger} | -1.7 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |

CA

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 8.6 | 4.0 | 4.4 | 4.4 | 4.4 | 4.4 |
| E_0 | 1.3 | 0.4 | 0.4 | 0.6 | 0.4 | 0.6 |
| E^{\dagger} | 30.6 | 13.8 | 14.9 | 14.6 | 14.9 | 14.6 |
| SH_0 | -2.4 | 0.1 | -1.0 | -1.0 | -1.0 | -1.0 |
| SH^{\dagger} | -2.0 | -2.0 | -2.0 | -1.5 | -2.0 | -1.5 |

Pyrimidine-purine (YR) base-pair steps (continued)

TG

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 8.2 | 3.8 | 4.2 | 4.2 | 4.2 | 4.2 |
| E_0 | 1.0 | 0.4 | 0.5 | 0.7 | 0.5 | 0.7 |
| E^\dagger | 29.1 | 13.1 | 14.5 | 14.3 | 14.5 | 14.3 |
| SH_0 | 0.1 | -2.4 | -2.4 | -1.0 | -2.4 | -1.0 |
| SH^\dagger | -1.7 | -1.7 | -1.7 | -1.9 | -1.7 | -1.9 |

TA

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 8.7 | 4.3 | 4.3 | 4.7 | 4.6 | 4.8 |
| E_0 | 1.0 | 0.6 | 0.7 | 0.8 | 0.7 | 0.8 |
| E^\dagger | 26.6 | 14.8 | 14.8 | 19.1 | 16.9 | 19.4 |
| SH_0 | -2.4 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| SH^\dagger | -1.9 | -1.5 | -1.5 | -1.5 | -1.5 | -1.5 |

(ii) Purine-purine and pyrimidine-pyrimidine (RR, YY) base-pair steps*AG*

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 18.1 | 9.4 | 10.7 | 11.1 | 10.7 | 11.1 |
| E_0 | 1.0 | 0.8 | 0.8 | 0.9 | 0.8 | 0.9 |
| E^\dagger | 67.1 | 33.4 | 41.8 | 44.0 | 41.9 | 44.0 |
| SH_0 | 1.0 | -0.1 | -0.1 | -0.1 | -0.1 | -0.1 |
| SH^\dagger | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |

CT

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 19.4 | 10.2 | 11.5 | 12.0 | 11.5 | 12.0 |
| E_0 | 0.6 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 |
| E^\dagger | 59.4 | 31.4 | 39.0 | 40.7 | 39.0 | 40.7 |
| SH_0 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| SH^\dagger | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |

Purine-purine and pyrimidine-pyrimidine (RR, YY) base-pair steps (continued)

GG

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 10.3 | 5.4 | 5.9 | 5.7 | 5.9 | 5.7 |
| E_0 | 0.9 | 0.5 | 0.4 | 0.3 | 0.4 | 0.3 |
| E^\dagger | 44.4 | 17.9 | 18.5 | 18.9 | 18.4 | 18.9 |
| SH_0 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| SH^\dagger | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 |

CC

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 11.4 | 6.0 | 6.5 | 6.6 | 6.5 | 6.6 |
| E_0 | 0.7 | 0.5 | 0.5 | 0.3 | 0.5 | 0.3 |
| E^\dagger | 39.0 | 18.2 | 18.9 | 17.8 | 18.9 | 17.8 |
| SH_0 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| SH^\dagger | -2.0 | -2.0 | -2.0 | -1.9 | -2.0 | -1.9 |

Purine-purine and pyrimidine-pyrimidine (RR, YY) base-pair steps (continued)

AA

| Score | Olson <i>et al.</i> * $\langle E \rangle$ | A+B+AB 13.8 | B+AB 12.3 | B 12.2 | B+AB+TA 11.5 | B+TA 11.6 |
|--------------|--|----------------|--------------|-----------|-----------------|--------------|
| E_0 | 1.4 | 1.2 | 1.2 | 1.2 | 0.9 | 0.9 |
| E^\dagger | 50.7 | 39.2 | 39.2 | 38.6 | 39.0 | 39.1 |
| SH_0 | 1.7 | 1.7 | 1.7 | 1.7 | 1.7 | 1.7 |
| SH^\dagger | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 | 1.5 |

TT

| Score | Olson <i>et al.</i> * $\langle E \rangle$ | A+B+AB 14.5 | B+AB 12.8 | B 12.8 | B+AB+TA 12.1 | B+TA 12.1 |
|--------------|--|----------------|--------------|-----------|-----------------|--------------|
| E_0 | 1.8 | 1.2 | 1.2 | 1.1 | 0.8 | 0.8 |
| E^\dagger | 45.8 | 37.5 | 37.5 | 37.4 | 37.7 | 38.4 |
| SH_0 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 |
| SH^\dagger | -1.6 | -1.6 | -1.6 | -1.6 | -1.6 | -1.6 |

Purine-purine and pyrimidine-pyrimidine (RR, YY) base-pair steps (continued)

GA

| Score | Olson <i>et al.</i> * $\langle E \rangle$ | A+B+AB E ₀ | B+AB E [†] | B SH ₀ | B+AB+TA SH [†] | B+TA |
|-------|--|--------------------------|------------------------|----------------------|----------------------------|------|
| | 12.3 | 7.5 | 7.5 | 8.7 | 7.5 | 8.7 |
| | 1.0 | 0.7 | 0.7 | 0.9 | 0.7 | 0.9 |
| | 47.3 | 24.6 | 24.4 | 31.7 | 24.4 | 31.7 |
| | -0.1 | -0.1 | -0.1 | -0.1 | -0.1 | -0.1 |
| | -1.7 | -1.5 | -1.5 | -1.5 | -1.5 | -1.5 |

TC

| Score | Olson <i>et al.</i> * $\langle E \rangle$ | A+B+AB E ₀ | B+AB E [†] | B SH ₀ | B+AB+TA SH [†] | B+TA |
|-------|--|--------------------------|------------------------|----------------------|----------------------------|------|
| | 13.5 | 8.0 | 8.1 | 9.4 | 8.1 | 9.4 |
| | 2.0 | 1.1 | 1.2 | 1.3 | 1.2 | 1.3 |
| | 45.7 | 25.7 | 25.8 | 30.4 | 25.8 | 30.4 |
| | -0.9 | 0.1 | 0.1 | -0.9 | 0.1 | -0.9 |
| | 2.5 | -1.6 | -1.6 | -1.6 | -1.6 | -1.6 |

(iii) Purine-pyrimidine (RY) base-pair steps

AT

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 26.0 | 15.6 | 16.6 | 18.4 | 16.5 | 18.4 |
| E_0 | 0.6 | 0.3 | 0.3 | 0.2 | 0.3 | 0.2 |
| E^\dagger | 79.0 | 45.4 | 49.8 | 56.0 | 50.7 | 56.0 |
| SH_0 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 |
| SH^\dagger | 1.5 | -2.0 | -2.0 | 1.5 | -2.0 | 1.5 |

AC

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 21.0 | 15.8 | 15.7 | 12.7 | 15.7 | 12.7 |
| E_0 | 1.0 | 0.8 | 0.7 | 0.6 | 0.8 | 0.6 |
| E^\dagger | 62.5 | 51.9 | 51.5 | 44.9 | 51.5 | 44.9 |
| SH_0 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 |
| SH^\dagger | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 |

Purine-pyrimidine (RY) base-pair steps (continued)

GT

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 20.3 | 15.6 | 15.6 | 12.5 | 15.6 | 12.5 |
| E_0 | 1.1 | 0.9 | 0.9 | 0.7 | 0.9 | 0.7 |
| E^\dagger | 62.4 | 44.1 | 44.1 | 38.4 | 44.1 | 38.4 |
| SH_0 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 | 1.2 |
| SH^\dagger | -2.0 | 1.5 | 1.5 | -2.0 | 1.5 | -2.0 |

GC

| Score | Olson <i>et al.</i> [*] | A+B+AB | B+AB | B | B+AB+TA | B+TA |
|---------------------|----------------------------------|--------|------|------|---------|------|
| $\langle E \rangle$ | 15.7 | 7.1 | 8.8 | 7.1 | 8.8 | 7.1 |
| E_0 | 1.9 | 1.0 | 1.1 | -1.9 | 1.1 | -1.9 |
| E^\dagger | 89.8 | 39.8 | 47.1 | 32.0 | 47.1 | 32.0 |
| SH_0 | 1.2 | 1.2 | 1.2 | -2.3 | 1.2 | -2.3 |
| SH^\dagger | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 | -2.0 |

[†] Knowledge-based scores — average cost $\langle E \rangle$ over the central 60 base-pair steps of the best-resolved nucleosome core particle structure (2) and the least and most costly values, E_0 and E^\dagger — derived from the base-pair step parameters of DNA dimers of different conformational types from high-resolution protein-DNA structures. Locations SH_0 and SH^\dagger of the least and most costly steps are expressed in terms of superhelical position, *i.e.*, number of helical turns with respect to the structural dyad. See text and legend to Table 1

*W.K. Olson, A.A. Gorin, X.-J. Lu, L.M. Hock & V.B. Zhurkin (1998) DNA sequence-dependent deformability deduced from protein-DNA crystal complexes, Proc. Natl. Acad. Sci., USA 95, 11163-11168.

Table S5. Threading scores of known nucleosome binding and antislection sequences on the central 60 base-pair steps of the 147-bp nucleosome core-particle structure (NDB_ID pd0287) (2) and an ideal 61-bp superhelical template with the same average global structure.[§]

| Sequence_ID | Crystallographic template | | | | Smooth superhelical template | | | |
|--|---------------------------|------------|-------|-------------|------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| Nucleosome-binding sequences from the mouse genome | | | | | | | | |
| <i>A-tracts 1</i> | | | | | | | | |
| phcn4 | 501 | 43 | 415 | 633 | 146 | 3 | 140 | 152 |
| phcn8 | 511 | 42 | 431 | 618 | 147 | 3 | 142 | 153 |
| phcn12 | 510 | 42 | 408 | 632 | 146 | 4 | 139 | 158 |
| phcn14 | 507 | 41 | 421 | 649 | 146 | 3 | 141 | 154 |
| phcn17 | 511 | 42 | 430 | 594 | 145 | 3 | 139 | 152 |
| phcn18 | 500 | 51 | 396 | 629 | 148 | 3 | 140 | 154 |
| phcn21 | 499 | 45 | 393 | 638 | 145 | 3 | 138 | 152 |
| phcn22 | 495 | 42 | 412 | 615 | 143 | 3 | 137 | 148 |
| phcn23 | 498 | 45 | 391 | 635 | 144 | 4 | 139 | 155 |
| phcn24 | 493 | 45 | 382 | 620 | 141 | 2 | 137 | 146 |
| phcn26 | 499 | 45 | 387 | 637 | 144 | 2 | 140 | 149 |
| phcn29 | 501 | 47 | 378 | 640 | 144 | 3 | 138 | 150 |
| phcn39 | 494 | 44 | 400 | 640 | 144 | 3 | 137 | 150 |
| phcn43 | 490 | 37 | 423 | 625 | 141 | 3 | 135 | 149 |
| phcn46 | 502 | 41 | 414 | 618 | 146 | 4 | 136 | 154 |
| phcn47 | 506 | 41 | 409 | 619 | 145 | 3 | 137 | 152 |
| phcn50 | 494 | 40 | 406 | 607 | 142 | 2 | 138 | 147 |
| phwn12 | 501 | 41 | 408 | 592 | 146 | 2 | 143 | 152 |
| <i>A-tracts 2</i> | | | | | | | | |
| phcn2 | 503 | 44 | 408 | 598 | 144 | 2 | 137 | 148 |
| phcn10 | 499 | 41 | 401 | 604 | 143 | 3 | 136 | 148 |
| phcn13 | 491 | 45 | 382 | 635 | 145 | 3 | 139 | 151 |
| phcn20 | 506 | 43 | 410 | 593 | 146 | 3 | 139 | 151 |
| phcn30 | 494 | 40 | 397 | 597 | 144 | 5 | 133 | 153 |
| phcn42 | 509 | 43 | 416 | 601 | 146 | 3 | 141 | 153 |
| phwn8 | 517 | 45 | 418 | 606 | 145 | 3 | 140 | 150 |
| phwn26 | 500 | 45 | 410 | 607 | 145 | 3 | 140 | 152 |

| Sequence_ID | Crystallographic template | | | | Smooth superhelical template | | | |
|--------------------|---------------------------|------------|-------|-------------|------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| phwn27 | 511 | 44 | 410 | 595 | 145 | 3 | 138 | 152 |
| <i>A-tracts 3</i> | | | | | | | | |
| phcn3 | 501 | 39 | 393 | 607 | 144 | 3 | 136 | 150 |
| phcn7 | 493 | 47 | 381 | 614 | 143 | 2 | 139 | 148 |
| phcn9 | 510 | 43 | 403 | 597 | 146 | 5 | 135 | 154 |
| phcn11 | 510 | 49 | 414 | 616 | 144 | 4 | 137 | 151 |
| phcn19 | 494 | 43 | 399 | 587 | 143 | 3 | 136 | 149 |
| phcn28 | 500 | 39 | 393 | 600 | 144 | 2 | 141 | 149 |
| phcn37 | 497 | 46 | 389 | 638 | 144 | 2 | 139 | 150 |
| phcn44 | 500 | 46 | 387 | 636 | 143 | 2 | 139 | 149 |
| phwn11 | 496 | 42 | 386 | 615 | 143 | 3 | 137 | 148 |
| phwn29 | 509 | 44 | 401 | 597 | 146 | 5 | 135 | 153 |
| phwn36 | 513 | 41 | 419 | 596 | 146 | 4 | 137 | 153 |
| <i>TG/CTG runs</i> | | | | | | | | |
| phcn31 | 531 | 40 | 446 | 619 | 161 | 5 | 150 | 170 |
| phcn32 | 535 | 58 | 417 | 623 | 163 | 4 | 151 | 171 |
| phcn33 | 550 | 47 | 452 | 621 | 168 | 4 | 161 | 176 |
| phcn40 | 527 | 32 | 458 | 642 | 155 | 6 | 144 | 168 |
| phwn2 | 496 | 42 | 416 | 589 | 148 | 4 | 140 | 158 |
| phwn3 | 518 | 36 | 449 | 622 | 151 | 5 | 140 | 162 |
| phwn4 | 498 | 42 | 421 | 590 | 149 | 3 | 141 | 157 |
| phwn7 | 461 | 33 | 380 | 555 | 137 | 5 | 128 | 148 |
| phwn10 | 525 | 50 | 427 | 609 | 154 | 3 | 147 | 162 |
| phwn13 | 536 | 58 | 414 | 644 | 161 | 3 | 156 | 167 |
| phwn14 | 527 | 51 | 381 | 611 | 156 | 7 | 136 | 166 |
| phwn15 | 560 | 50 | 457 | 656 | 169 | 2 | 163 | 176 |
| phwn16 | 499 | 43 | 422 | 614 | 145 | 5 | 134 | 155 |
| phwn17 | 502 | 39 | 396 | 584 | 150 | 6 | 136 | 163 |
| phwn18 | 495 | 50 | 401 | 602 | 144 | 4 | 134 | 152 |
| phwn20 | 495 | 41 | 409 | 589 | 143 | 3 | 135 | 151 |
| phwn22 | 508 | 33 | 430 | 595 | 151 | 5 | 141 | 162 |
| phwn23 | 528 | 43 | 427 | 650 | 159 | 4 | 152 | 169 |
| phwn24 | 507 | 37 | 432 | 615 | 147 | 6 | 136 | 162 |

| Sequence_ID | Crystallographic template | | | | Smooth superhelical template | | | |
|---------------------|---------------------------|------------|-------|-------------|------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| phwn25 | 492 | 44 | 385 | 581 | 145 | 6 | 132 | 157 |
| phwn28 | 506 | 36 | 433 | 621 | 146 | 6 | 136 | 158 |
| phwn30 | 495 | 36 | 409 | 597 | 147 | 4 | 138 | 157 |
| phwn32 | 479 | 38 | 407 | 561 | 146 | 7 | 132 | 156 |
| <i>Phased TATA</i> | | | | | | | | |
| phcn5 | 502 | 38 | 436 | 589 | 146 | 13 | 127 | 173 |
| phcn25 | 513 | 36 | 431 | 582 | 147 | 11 | 131 | 170 |
| phcn41 | 509 | 38 | 415 | 583 | 149 | 12 | 131 | 171 |
| phcn49 | 520 | 41 | 430 | 610 | 152 | 12 | 133 | 174 |
| <i>Phased TG/CA</i> | | | | | | | | |
| phcn6 | 528 | 43 | 434 | 636 | 156 | 3 | 147 | 163 |
| phcn16 | 523 | 47 | 405 | 622 | 155 | 3 | 147 | 159 |
| phcn27 | 530 | 46 | 417 | 628 | 156 | 2 | 150 | 160 |
| phcn48 | 529 | 47 | 447 | 642 | 154 | 2 | 148 | 158 |
| <i>No sequence</i> | | | | | | | | |
| phcn1 | 483 | 33 | 407 | 567 | 141 | 4 | 132 | 149 |
| phcn15 | 492 | 39 | 420 | 574 | 142 | 5 | 129 | 152 |
| phcn34 | 511 | 39 | 436 | 598 | 147 | 5 | 137 | 157 |
| phcn35 | 467 | 35 | 371 | 581 | 133 | 5 | 123 | 146 |
| phcn36 | 493 | 41 | 385 | 597 | 144 | 7 | 123 | 155 |
| phcn38 | 467 | 35 | 371 | 581 | 133 | 5 | 123 | 146 |
| phcn45 | 470 | 38 | 382 | 593 | 134 | 7 | 121 | 148 |
| phwn1 | 467 | 32 | 383 | 535 | 136 | 6 | 123 | 149 |
| phwn5 | 491 | 43 | 410 | 582 | 141 | 5 | 132 | 151 |
| phwn6 | 465 | 34 | 387 | 540 | 135 | 7 | 119 | 155 |
| phwn9 | 473 | 40 | 397 | 566 | 136 | 4 | 127 | 146 |
| phwn19 | 498 | 38 | 420 | 603 | 144 | 4 | 137 | 152 |
| phwn21 | 477 | 39 | 379 | 562 | 134 | 5 | 120 | 145 |
| phwn31 | 494 | 46 | 386 | 597 | 142 | 5 | 132 | 152 |
| phwn33 | 471 | 38 | 394 | 584 | 141 | 8 | 126 | 158 |
| phwn34 | 503 | 39 | 385 | 595 | 143 | 5 | 134 | 153 |
| phwn35 | 467 | 36 | 386 | 560 | 131 | 8 | 116 | 147 |
| phwn37 | 450 | 27 | 393 | 528 | 133 | 5 | 121 | 143 |

| Sequence_ID | Crystallographic template | | | | Smooth superhelical template | | | |
|---|---------------------------|------------|-------|-------------|------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| Anti-selection sequences from the mouse genome | | | | | | | | |
| <i>TGGA fragments</i> | | | | | | | | |
| 35 | 500 | 25 | 442 | 541 | 154 | 3 | 148 | 158 |
| 19 | 492 | 35 | 431 | 576 | 153 | 2 | 148 | 156 |
| 29 | 480 | 39 | 397 | 566 | 149 | 3 | 143 | 156 |
| 75 | 495 | 50 | 410 | 600 | 152 | 2 | 149 | 158 |
| 44 | 486 | 34 | 413 | 567 | 146 | 3 | 140 | 154 |
| 81 | 482 | 35 | 416 | 569 | 149 | 3 | 143 | 154 |
| 49 | 474 | 31 | 426 | 528 | 147 | 3 | 143 | 152 |
| 62 | 474 | 44 | 374 | 566 | 148 | 2 | 144 | 152 |
| 57 | 472 | 32 | 408 | 548 | 147 | 2 | 143 | 152 |
| 47 | 480 | 41 | 369 | 571 | 146 | 2 | 140 | 150 |
| 77 | 481 | 40 | 404 | 566 | 149 | 3 | 142 | 155 |
| 23 | 478 | 42 | 397 | 572 | 146 | 3 | 140 | 152 |
| 80 | 482 | 31 | 433 | 557 | 149 | 2 | 146 | 153 |
| 86 | 463 | 43 | 371 | 566 | 144 | 2 | 140 | 151 |
| <i>Badsecs</i> | | | | | | | | |
| 24 | 490 | 31 | 424 | 562 | 144 | 5 | 133 | 154 |
| 26 | 498 | 33 | 446 | 569 | 142 | 1 | 140 | 145 |
| 28 | 511 | 51 | 418 | 653 | 148 | 3 | 143 | 152 |
| 48 | 502 | 36 | 420 | 582 | 145 | 6 | 134 | 160 |
| 51 | 500 | 33 | 418 | 564 | 140 | 4 | 133 | 148 |
| 78 | 503 | 34 | 397 | 556 | 146 | 6 | 134 | 157 |
| 31 | 508 | 41 | 432 | 571 | 147 | 3 | 140 | 152 |
| 32 | 516 | 49 | 427 | 627 | 149 | 3 | 140 | 154 |
| 33 | 518 | 38 | 424 | 597 | 149 | 8 | 129 | 163 |
| 52 | 494 | 30 | 428 | 551 | 143 | 6 | 133 | 153 |
| 63 | 526 | 36 | 433 | 595 | 147 | 7 | 138 | 161 |
| 69 | 508 | 37 | 454 | 615 | 146 | 4 | 131 | 153 |
| 73 | 506 | 35 | 428 | 589 | 146 | 4 | 139 | 156 |
| 76 | 493 | 34 | 430 | 593 | 144 | 4 | 135 | 152 |
| 84 | 486 | 27 | 433 | 544 | 144 | 6 | 134 | 157 |
| 85 | 503 | 34 | 418 | 594 | 149 | 4 | 141 | 157 |

| Sequence_ID | <i>Crystallographic template</i> | | | | <i>Smooth superhelical template</i> | | | |
|----------------------------------|----------------------------------|------------|-------|-------------|-------------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| 27 | 452 | 38 | 386 | 532 | 128 | 4 | 119 | 138 |
| 30 | 490 | 38 | 395 | 559 | 142 | 4 | 134 | 148 |
| 43 | 484 | 35 | 389 | 579 | 136 | 4 | 130 | 142 |
| 53 | 488 | 30 | 437 | 549 | 140 | 4 | 132 | 147 |
| 55 | 489 | 36 | 422 | 556 | 142 | 3 | 135 | 146 |
| 56 | 493 | 28 | 450 | 538 | 142 | 6 | 133 | 149 |
| 59 | 485 | 49 | 397 | 593 | 142 | 4 | 134 | 151 |
| 66 | 515 | 42 | 397 | 616 | 147 | 5 | 138 | 156 |
| 67 | 521 | 48 | 444 | 602 | 152 | 4 | 141 | 158 |
| 74 | 512 | 40 | 432 | 602 | 143 | 4 | 137 | 151 |
| Synthetic SELEX sequences | | | | | | | | |
| 10nvp | 477 | 32 | 407 | 561 | 136 | 5 | 121 | 150 |
| 11nvp | 483 | 41 | 390 | 579 | 137 | 5 | 126 | 149 |
| 13nvp | 467 | 36 | 368 | 615 | 132 | 7 | 114 | 146 |
| 16nvp | 488 | 36 | 371 | 595 | 139 | 6 | 124 | 151 |
| 18nvp | 479 | 40 | 362 | 611 | 138 | 5 | 127 | 149 |
| 22nvp | 480 | 38 | 376 | 577 | 138 | 6 | 124 | 153 |
| 24nvp | 481 | 34 | 364 | 575 | 139 | 5 | 122 | 148 |
| 25nvp | 479 | 41 | 368 | 629 | 139 | 5 | 128 | 152 |
| 26nvp | 493 | 38 | 397 | 589 | 141 | 7 | 124 | 155 |
| 28nvp | 485 | 40 | 368 | 597 | 140 | 7 | 124 | 155 |
| 29nvp | 484 | 42 | 390 | 609 | 140 | 6 | 124 | 150 |
| 2nvp | 490 | 38 | 400 | 630 | 140 | 4 | 130 | 147 |
| 30nvp | 481 | 31 | 416 | 572 | 138 | 5 | 126 | 154 |
| 34nvp | 483 | 41 | 345 | 584 | 138 | 4 | 128 | 148 |
| 37nvp | 471 | 38 | 359 | 586 | 138 | 5 | 126 | 149 |
| 38nvp | 471 | 42 | 382 | 605 | 136 | 5 | 122 | 148 |
| 40nvp | 469 | 41 | 345 | 601 | 134 | 6 | 122 | 152 |
| 41nvp | 477 | 37 | 399 | 562 | 136 | 4 | 125 | 150 |
| 52nvp | 481 | 38 | 378 | 589 | 137 | 5 | 123 | 146 |
| 54nvp | 484 | 41 | 393 | 643 | 138 | 7 | 123 | 155 |
| 5nvp | 483 | 38 | 394 | 599 | 140 | 4 | 128 | 151 |
| 602nvp_rev_rev | 477 | 37 | 382 | 573 | 136 | 7 | 124 | 154 |

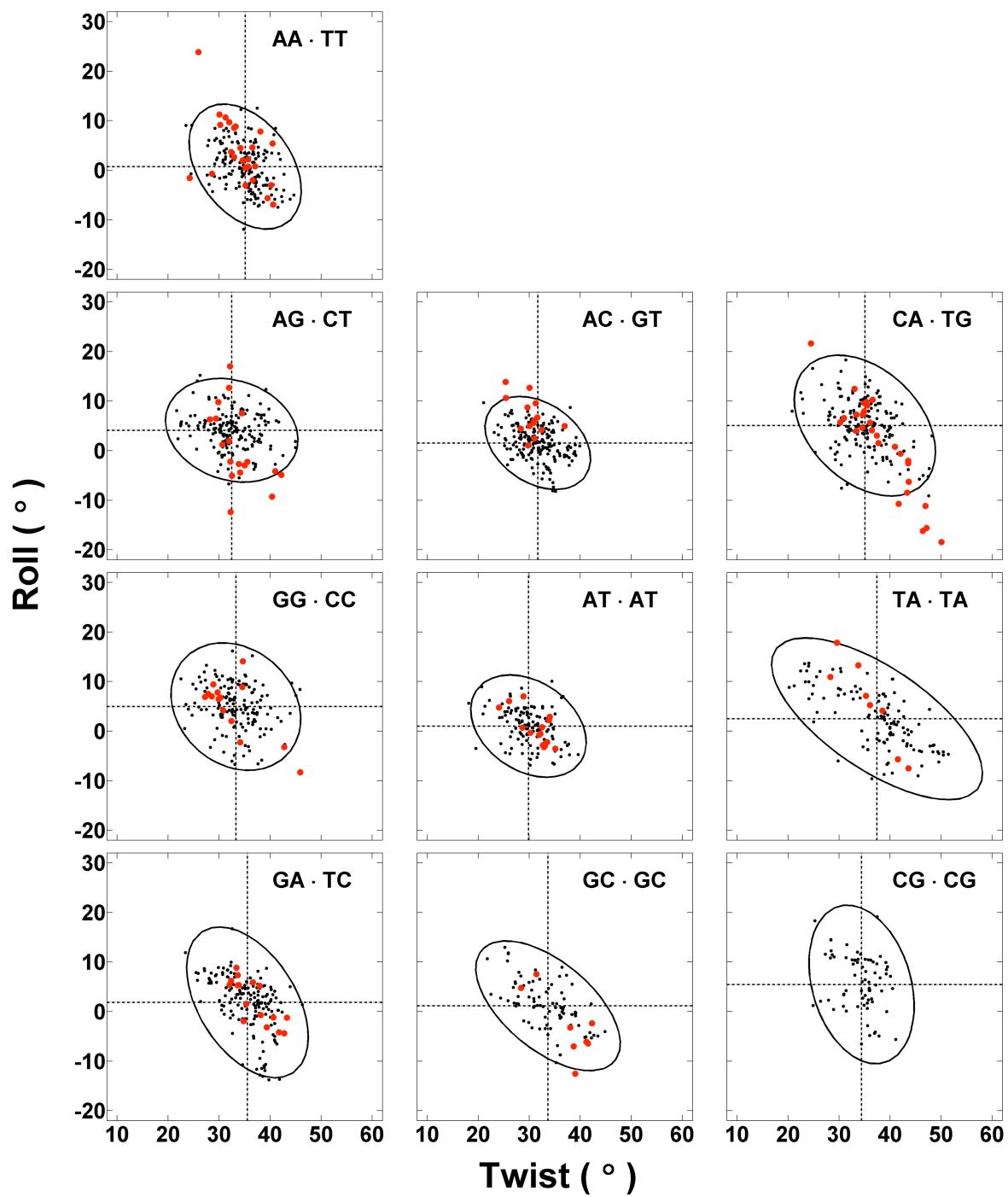
| Sequence_ID | <i>Crystallographic template</i> | | | | <i>Smooth superhelical template</i> | | | |
|----------------|----------------------------------|------------|-------|-------------|-------------------------------------|------------|-------|-------------|
| | $\langle U \rangle$ | σ_U | U_0 | U^\dagger | $\langle U \rangle$ | σ_U | U_0 | U^\dagger |
| 603nvp | 487 | 44 | 358 | 618 | 138 | 5 | 124 | 150 |
| 604rnvp | 496 | 37 | 415 | 594 | 141 | 5 | 129 | 154 |
| 605nvp | 489 | 39 | 371 | 575 | 139 | 5 | 126 | 153 |
| 607nvp_rev_rev | 476 | 39 | 347 | 571 | 135 | 4 | 123 | 146 |
| 609nvp | 475 | 41 | 381 | 587 | 136 | 7 | 118 | 152 |
| 611nvp | 466 | 37 | 361 | 585 | 132 | 5 | 121 | 143 |
| 613nvp | 476 | 41 | 372 | 583 | 138 | 5 | 126 | 149 |
| 615fnvp | 475 | 39 | 342 | 590 | 134 | 6 | 123 | 152 |
| 618nvp_rev_rev | 479 | 37 | 390 | 587 | 137 | 4 | 128 | 146 |
| 620nvp_rev_rev | 470 | 40 | 366 | 577 | 133 | 5 | 121 | 146 |
| 621rnvp | 480 | 36 | 390 | 565 | 137 | 5 | 125 | 152 |
| 624bnvp | 481 | 36 | 389 | 570 | 137 | 4 | 129 | 145 |
| 626nvp | 488 | 34 | 399 | 579 | 139 | 5 | 126 | 150 |
| 628nvp_rev_rev | 477 | 43 | 374 | 586 | 136 | 8 | 117 | 157 |
| 69nvp | 475 | 44 | 373 | 610 | 135 | 7 | 119 | 149 |
| 6nvp | 474 | 39 | 386 | 576 | 134 | 5 | 122 | 149 |
| 73nvp | 485 | 44 | 358 | 628 | 139 | 5 | 123 | 148 |
| 7nvp | 485 | 35 | 408 | 593 | 137 | 5 | 128 | 149 |
| 83nvp | 472 | 42 | 340 | 630 | 137 | 6 | 123 | 152 |

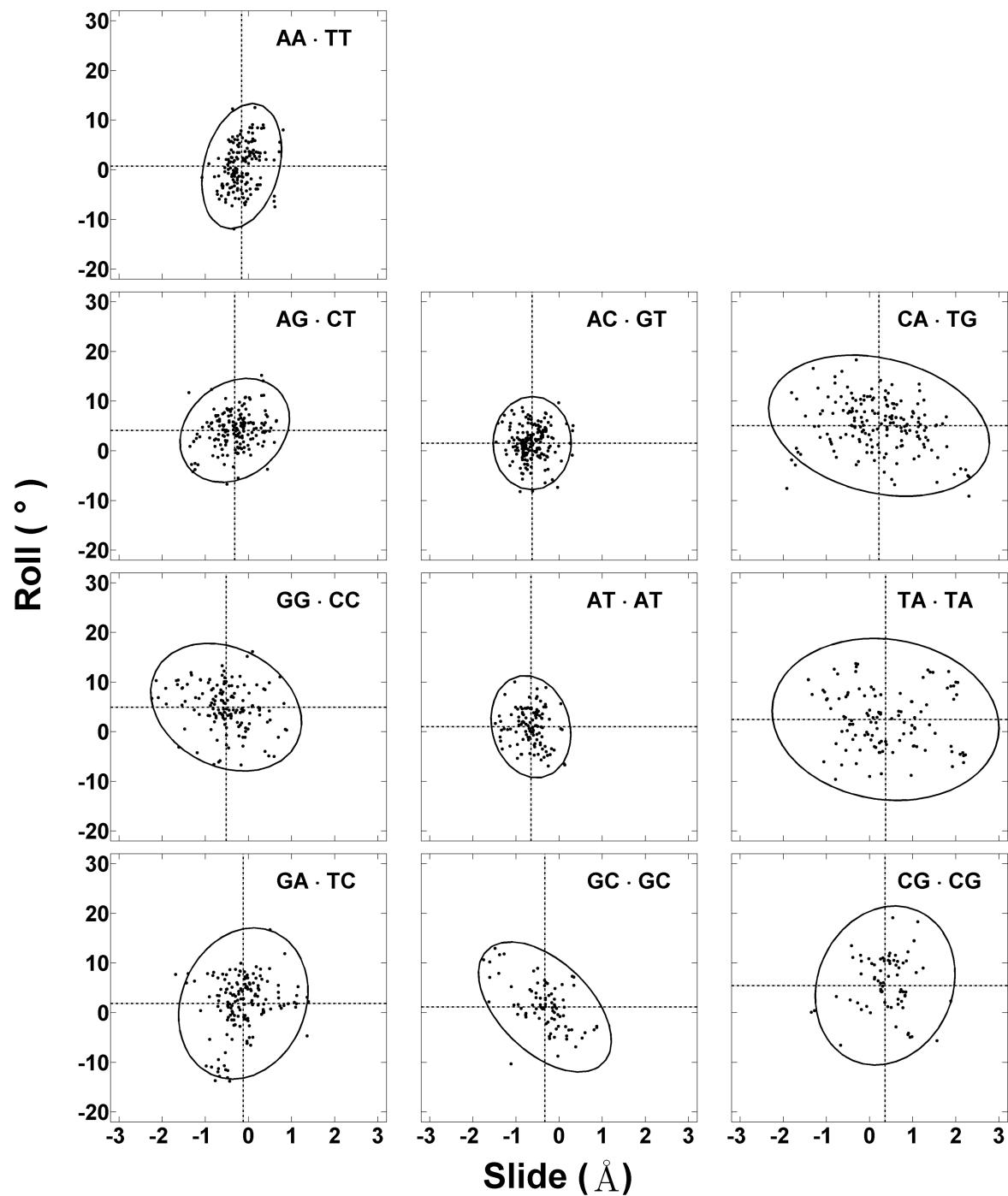
[§] Threading scores reported for individual sequences are the total dimeric scores computed with Eqn. (1) using all six step parameters and elastic constants and rest states based on the dimer steps from all conformational categories, *i.e.*, the A+B+AB dataset in Table 1. Values include the mean score $\langle U \rangle$ and the standard deviation σ_U for all possible settings of each sequence on the designated templates as well as the lowest and highest scores U_0 and U^\dagger associated with the best and worst settings of each sequence on the template.

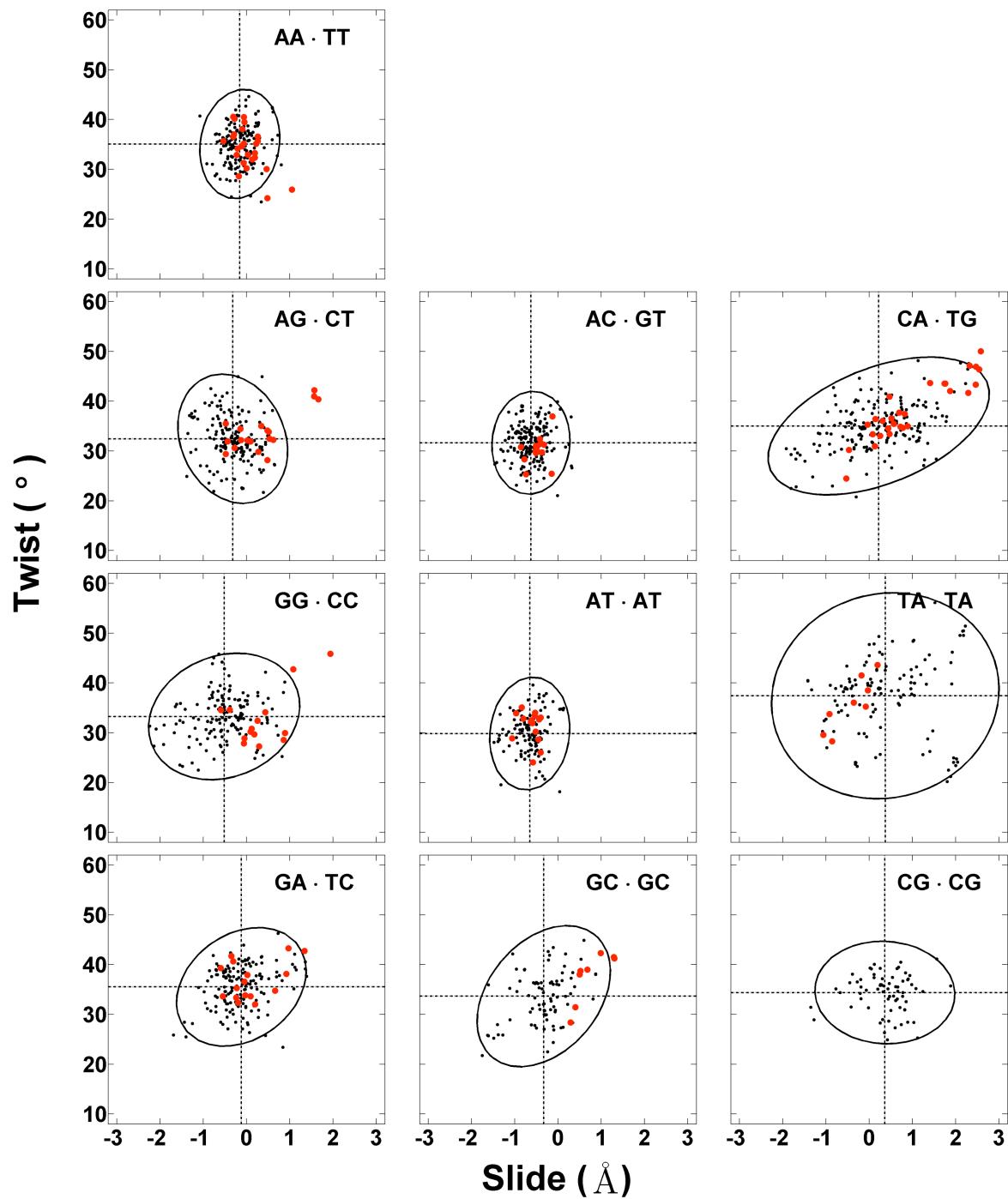
Legends to Supplementary Figures

Figure S1. Collective scatter plots of the rigid-body (step) parameters found for the ten unique DNA base-pair steps in the high-resolution protein-DNA crystal complexes that make up the reference database, the sequence-dependent potentials derived from these data, and the step-parameter values found in nucleosomal DNA. Small black dots correspond to the points used to derive the potentials (solid contours) and large red dots to the states that the given dimers adopt in the currently best-resolved nucleosome core particle structure (NDB_ID pd0287, Davey *et al.* 2002. *J. Mol. Biol.* **319**, 1097-1113). Ellipses are projections of the multi-dimensional potentials on the specified conformational planes obtained from the 2×2 covariance matrices of observed values: (a) Roll-Twist; (b) Roll-Slide; (c) Twist-Slide. Contours correspond to deviations of parameters equal to two times the combined root-mean-square deviations from the intrinsic (mean) values. Average values of step parameters are highlighted by thin (dashed) lines. The three columns show the respective deformational patterns of individual purine-purine (RR), purine-pyrimidine (RY), and pyrimidine-purine (YR) steps. Note the absence of CG steps in the nucleosomal DNA. Images kindly provided by Guohui Zheng.

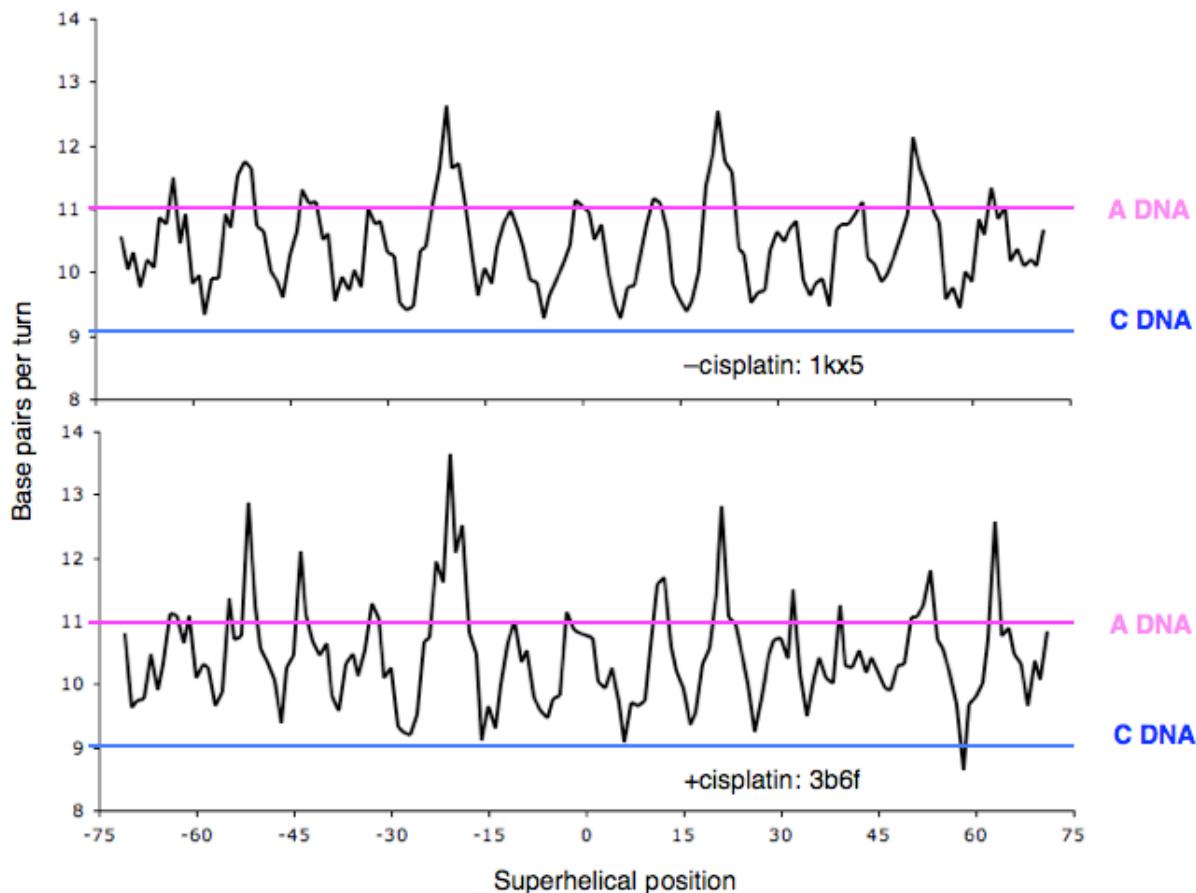
Figure S2. Comparative variation of Twist, expressed as the number of base pairs that would form a complete turn of an ideal, naturally straight helix, as a function of DNA superhelical position in two 147-bp nucleosome core-particle structures: (top) the DNA pathway in the currently best-resolved nucleosome core particle structure (NDB_ID pd0287/PDB_ID 1kx5, Davey *et al.* 2002. *J. Mol. Biol.* **319**, 1097-1113); (bottom) the pathway adopted by the same sequence in the presence of cisplatin (NDB_ID pd1046/PDB_ID 3b6f, Wu & Davey. 2008. *Nature Chem. Biol.* **4**, 110-112). Superhelical positions correspond to the number of double-helical turns a dimeric step is displaced from the structural dyad on the central base pair (here denoted by 0). Color-coded lines denote the helical repeat in the canonical A-DNA (Franklin & Gosling. 1953. *Nature* **171**, 740-741) and C-DNA (Marvin *et al.* 1958. *Nature* **182**, 387-388) double helices.

Balasubramanian *et al.*, Figure S1a

Balasubramanian *et al.*, Figure S1b

Balasubramanian *et al.*, Figure S1c

The presence of cisplatin appears to unwind nucleosomal DNA to more A-like states.



Balasubramanian *et al.*, Figure S2